



Degree Based Multiplicative Connectivity Indices of Nanostructures

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ABSTRACT

The Multiplicative topological indices of Phenyleneic, Naphatalenic, Anthracene and Tetracenic Nanotubes are calculated. The indices like Multiplicative Zagreb, Multiplicative Hyper-Zagreb, Multiplicative Sum connectivity, Multiplicative product connectivity, General multiplicative Zagreb, Multiplicative ABC and Multiplicative GA indices are expressed as a closed formula for the known values of s, t . The proposed formulae will be very useful for the study of nanostructure in the field of nanotechnology.

Keywords:

Topological indices, Molecular graphs, degree based topological index, Phenyleneic, multiplicative indices, Naphatalenic, Anthracene and Tetracenic nanotubes

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1. Introduction

A molecular graph is defined as a simple graph in which the vertices represent the atoms and the edges represent the bonds between the atoms. Graph theory is a developing branch of Mathematics. From the Mathematical modeling of the chemical compound, we can apply the graph theory concepts to the graphs of chemical structure. The application of graph theory is a powerful tool for studying in QSPR and QSAR. Topological indices are invariant values given by the structure of chemical compounds, which correlates with their physic-chemical properties. Phenyleneic nanotubes have cycles of length 4, 6 and 8. The cycles are arranged in the alternating manner. The structure of nanotubes is either a cylinder or in the form of a torus. Naphatalenic nanotubes have cycles of length 4, 6 and 8. The first row of the Naphatalenic nanotubes contains only C_4 and C_6 . Similarly, the second row contains the sequences of cycles of

length 6 and 8. So we can say that it is a lattice containing the cycles of length 4, 6 and 8, and it is a plane. The entire structure can cover either a cylinder or torus. Anthracene is denoted by the formula $C_{14}H_{10}$, which is a solid polycyclic aromatic hydrocarbon. It consists of 3 benzene rings which are fused. It is also known as cool tar. It is used in the production of dyes like red alizarin. Tetracenic is also a polycyclic aromatic hydrocarbon. It appeared to be orange powder light in color. The chemical graphs of Phenyleneic, Naphatalenic, Anthracene and Tetracenic Nanotubes are shown in the Figures 1, 2, 3 and 4.

Let H denotes the given graph. The set of vertices represented by $V(H)$ and the set of edges represented by $E(H)$. Also $d_H(v)$ be the degree of vertex v which is the number of vertices adjacent to v . The indices formulas are listed below as a ready reckoned for the calculation of multiplicative invariants.

Name of the Multiplicative indices	Formulae	Reference Number
First multiplicative Zagreb index	$II_1(H) = \prod_{u \in E(H)} d_H(u)^2,$	Todeshine <i>et. al.</i> (2010), Gutman (2011)
Second multiplicative Zagreb index	$II_2(H) = \prod_{uv \in E(H)} d_H(u)d_H(v).$	Todeshine <i>et. al.</i> (2010), Gutman (2011)

New multiplicative version of the first Zagreb index	$II_1^*(H) = \prod_{uv \in E(H)} [d_H(u) + d_H(v)]$	Eliasi <i>et. al.</i> (2012)
First multiplicative hyper-Zagreb index	$HII_1(H) = \prod_{uv \in E(H)} [d_H(u) + d_H(v)]^2$	Kulli (2016a)
Second multiplicative hyper-Zagreb index	$HII_2(H) = \prod_{uv \in E(H)} [d_H(u)d_H(v)]^2.$	Kulli (2016a)
General first multiplicative Zagreb index	$MZ_1^a(H) = \prod_{uv \in E(H)} [d_H(u) + d_H(v)]^a$	Kulli
General second multiplicative Zagreb index	$MZ_2^a(H) = \prod_{uv \in E(H)} [d_H(u)d_H(v)]^a$	Kulli
Randic index	$\chi(H) = \sum_{uv \in E(H)} \frac{1}{\sqrt{d_H(u)d_H(v)}}.$	Randic (1975)
Multiplicative sum connectivity index	$XII(H) = \prod_{uv \in E(H)} \frac{1}{\sqrt{d_H(u) + d_H(v)}}.$	Kulli (2016b)
Multiplicative product connectivity index	$\chi II(H) = \prod_{uv \in E(H)} \frac{1}{\sqrt{d_H(u)d_H(v)}}.$	Kulli (2016b)
Multiplicative atom bond connectivity index	$ABCII(H) = \prod_{uv \in E(H)} \sqrt{\frac{d_H(u) + d_H(v) - 2}{d_H(u)d_H(v)}}.$	Kulli (2016b)
Multiplicative geometric-arithmetic index	$GAII(H) = \prod_{uv \in E(H)} \frac{2\sqrt{d_H(u)d_H(v)}}{d_H(u) + d_H(v)}$	Kulli (2016b)
General multiplicative geometric-arithmetic index	$GA^a II(H) = \prod_{uv \in E(H)} \left(\frac{2\sqrt{d_H(u)d_H(v)}}{d_H(u) + d_H(v)} \right)^a$	Kulli (2016b)

Many literatures (Veylaki *et. al.* 2015), (Wei Gao 2017), (Farahani 2015), (Kulli 2018), (Imran Nadeem *et. al.* 2016), (Liu *et. al.* 2016), (Wei Geo *et. al.* 2017) are available in the study of topological indices based on additive and multiplicative indices. Recently these topological invariants of nanotubes correlates perfectly with the properties of nanotubes (Doslic *et. al.* 2011), (Vukicevic *et. al.* 2011), (Diudea 2010), (Diudea 2006). Therefore, the studies of four different types of nanotubes are selected and their topological invariants are computed and explained with their structures to the field of nanotechnology.

2. Results and Discussion

2.1 Results for V-Phenylenic nanotubes (V_p)

This type of nanotubes is defined as $VPHX[s, t]$. Here s- number of joining hexagons in row first and t -number

of another hexagons in column first. These nanotubes are defined in figure 1.

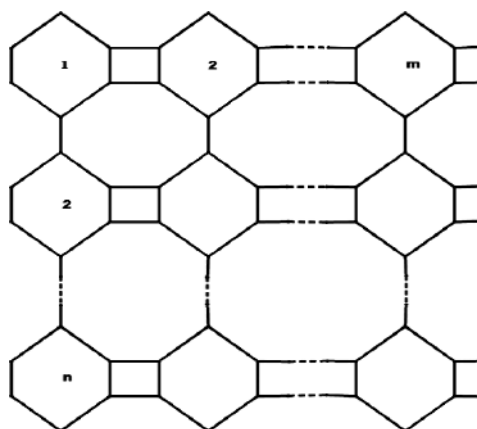


Figure 1

Lemma 2.1. Let $VPHX[s, t]$ is the V-Phenylic nanotubes, the vertex cardinality is $|V(P)| = 6st$. ($s, t > 1$).

Lemma 2.2 Let $VPHX[s, t]$ is the V-Phenylic nanotubes, the edge cardinality is $|E(P)| = 9st - s$. ($s, t > 1$).

Table 1: The following table shows the edges partitions by degrees of every edge in Phenylic nanotubes.

$d(a), d(b)$ where $ab \in E(P)$	$ E_2 $	$ E_3 $
Total edges	$4s$	$9st - 5s$

2.2 Results for V-Naphatalenic Nanotubes (V_N)

This type of nanotubes is defined as $NPHX[s, t]$. Here s-number of joining hexagons in row first and t-number of another hexagons in column first. These nanotubes are defined in figure 2.

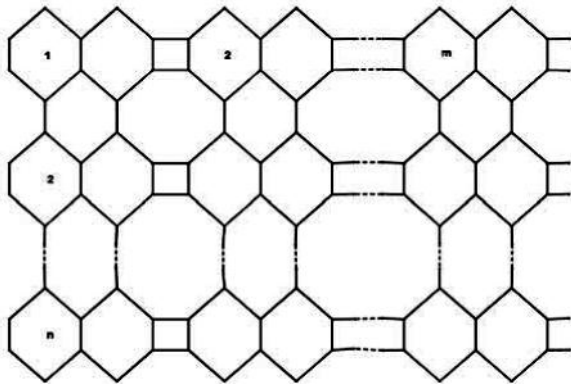


Figure 2

Lemma 2.3. Let $VPHX[s, t]$ is the N-Naphatalenic nanotubes, the vertex cardinality is $|V(N)| = 10st$. ($s, t > 1$)

Lemma 2.4 Let $VPHX[s, t]$ is the N-Naphatalenic nanotubes, the edge cardinality is $|E(N)| = 15st - 2s$. ($s, t > 1$).

Table 2: The following table shows the edges partitions by degrees of every edge in Naphatalenic nanotubes.

$d(a), d(b)$ where $ab \in E(N)$	$ E_2 $	$ E_3 $
Total edges	$8s$	$15st - 10s$

2.3 Results for V-Anthracene Nanotubes (V_A)

This type is defined as Anthracene $[s, t]$. Here s- number of joining hexagons in row first and t -number of another hexagons in column first. These nanotubes are defined in figure 3.

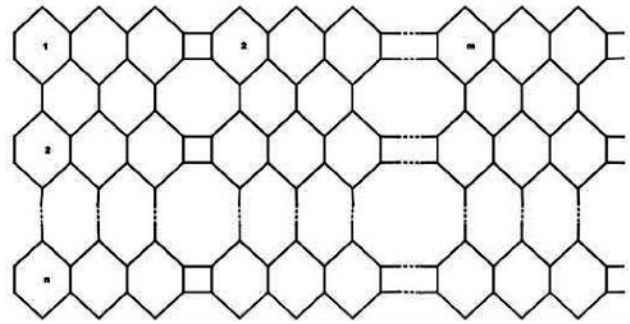


Figure 3

Lemma 2.5. Let V-Anthracene nanotubes, the vertex cardinality is $|V(A)| = 14st$. ($s, t > 1$).

Lemma 2.6. Let V-Anthracene nanotubes, the edge cardinality is $|E(A)| = 21st - 3s$. ($s, t > 1$).

Table 3: The following table shows the edges partitions by degrees of every edge in Anthracene nanotubes.

$d(a), d(b)$ where $ab \in E(A)$	$ E_2 $	$ E_3 $
Total edges	$12s$	$12st - 15s$

2.4 Results for V-Tetracenic (V_T)

This type is defined Tetracenic $[s, t]$. Here s-number of joining hexagons in row first and t -number of another hexagons in column first. These nanotubes are defined in figure 4.

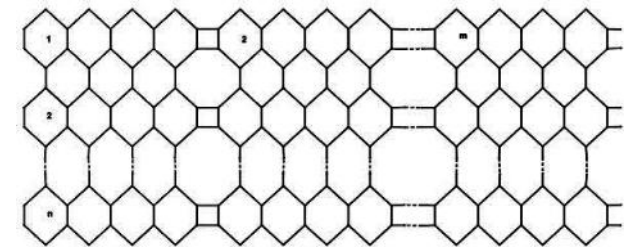


Figure 4

Lemma 2.7. Let V-Tetracenic nanotubes, the vertex cardinality is $|V(T)| = 18st$. ($s, t > 1$).

Lemma 2.8. Let V-Tetracenic nanotubes, the edge cardinality is $|E(T)| = 27st - 4s$. ($s, t > 1$).

Table 4: The following table shows the edges partitions by degrees of every edge in Tetracenic nanotubes

$d(a), d(b)$ where $ab \in E(T)$	$ E_2 $	$ E_3 $
Total edges	$16s$	$27st - 20s$

Table 5: Computing number of edges and vertices based on Hexagons:

Nanostructure	R	$ V $	$ E $	$ E_2 $	$ E_3 $
V-Phenylenic	1	$6st$	$9st - s$	$4s$	$9st - 5s$
V-Naphatalenic	2	$10st$	$15st - 2s$	$8s$	$15st - 10s$
V-Anthracene	3	$14st$	$21st - 3s$	$12s$	$21st - 15s$
V-Tetracenic	4	$18st$	$27st - 4s$	$16s$	$27st - 20s$

Generalizing the results by using an algebraic method, we obtain $|V| = (4R + 2)st$, $|E| = (6R + 3)st - sR$, $|E_2| = 4sR$ and $|E_3| = (6R + 3)st - 5sR$. Here R denotes the Number of Hexagons in the corresponding rows also columns in the nanotubes mentioned above.

Theorem 2.9. Let H be 2-dimensional lattice of any of the nanostructure (Phenylenic, Naphatalenic, Anthracene and Tetracenic). Then,

- (1). $II_1^*(H) = 5^{4sR} \times 6^{(6R+3)st-5sR}$
- (2). $II_2(H) = 2^{4sT} \times 3^{(6R+3)2st-6sR}$
- (3). $HII_1(H) = 5^{8sR} \times 6^{(6R+3)2st-10sR}$
- (4). $HII_2(H) = 2^{8sR} \times 3^{(6R+3)4st-12sR}$
- (5). $XII(H) = \left(\frac{1}{5}\right)^{2sR} \times \left(\frac{1}{\sqrt{6}}\right)^{(6R+3)st-5sR}$
- (6). $\chi II(H) = 2^{-2sR} \times 3^{3sR-(6R+3)st}$

- (7). $MZ_1^a(H) = 5^{4sRa} \times 6^{(6R+3)sta-5sRa}$
- (8). $MZ_2^a(H) = 2^{4sRa} \times 3^{(6R+3)2sta-6sRa}$
- (9). $ABCII(H) = 2^{(6R+3)st-7sR} \times 3^{5sR-(6R+3)st}$

$$(10). GAI(H) = \left(\frac{2\sqrt{6}}{5}\right)^{4sR}$$

$$(11). GA^a II(H) = \left(\frac{2\sqrt{6}}{5}\right)^{4saR}$$

Proof. By using the definitions of multiplicative indices and the proposed results from the table5, we get the following results:

$$(1). II_1^*(H) = \prod_{uv \in E(H)} [d_H(u) + d_H(v)] = \prod_{uv \in E_2} 5 \times \prod_{uv \in E_3} 6 = 5^{4sR} \times 6^{(6R+3)st-5sR}$$

Inference 1

Nanostructure	V-Phenylenic	V-Naphatalenic	V-Anthracene	V-Tetracenic
$II_1^*(H)$	$5^{4s} \times 6^{9st-5s}$	$5^{8s} \times 6^{15st-10s}$	$5^{12s} \times 6^{21st-15s}$	$5^{16s} \times 6^{27st-20s}$

$$(2). II_2(H) = \prod_{uv \in E(H)} d_H(u)d_H(v) = \prod_{uv \in E_2} 6 \times \prod_{uv \in E_3} 9 = 6^{4sR} \times 9^{(6R+3)st-5sR} = 2^{4sR} \times 3^{(6R+3)2st-6sR}$$

Inference 2

Nanostructure	V-Phenylenic	V-Naphatalenic	V-Anthracene	V-Tetracenic
$II_2(H)$	$2^{4s} \times 3^{18st-6s}$	$2^{8s} \times 3^{30st-12s}$	$2^{12s} \times 3^{42st-18s}$	$2^{16s} \times 3^{54st-24s}$

$$(3).a HII_1(H) = \prod_{uv \in E(H)} [d_H(u) + d_H(v)]^2 = \prod_{uv \in E_2} 5^2 \times \prod_{uv \in E_3} 6^2$$

$$= 5^{2(4sR)} \times 6^{2[(6R+3)st-5sR]} = 5^{8sR} \times 6^{(6R+3)2st-10sR}$$

Inference 3

Nanostructure	V-Phenylenic	V-Naphatalenic	V-Anthracene	V-Tetracenic
$HII_1(H)$	$5^{8s} \times 6^{18st-10s}$	$5^{16s} \times 6^{30st-20s}$	$5^{24s} \times 6^{42st-30s}$	$5^{32s} \times 6^{54st-40s}$

$$(4). \quad HII_2(H) = \prod_{uv \in E(H)} [d_H(u)d_H(v)]^2 = 6^{2(4sR)} \times 9^{2[(6R+3)st-5sR]}$$

$$= \prod_{uv \in E_2} 6^2 \times \prod_{uv \in E_3} 9^2 = 2^{8sR} \times 3^{(6R+3)4st-12sR}$$

Inference 4

Nanostructure	V-Phenylenic	V-Naphatalenic	V-Anthracene	V-Tetracenic
$HII_2(H)$	$2^{8s} \times 3^{36st-12s}$	$2^{16s} \times 3^{60st-24s}$	$2^{24s} \times 3^{84st-36s}$	$2^{32s} \times 3^{108st-48s}$

$$(5). \quad XII(H) = \prod_{uv \in E(H)} \frac{1}{\sqrt{d_H(u) + d_H(v)}} = \left(\frac{1}{\sqrt{5}}\right)^{4sR} \times \left(\frac{1}{\sqrt{6}}\right)^{(6R+3)st-5sR}$$

$$= \prod_{uv \in E_1} \frac{1}{\sqrt{4}} \times \prod_{uv \in E_2} \frac{1}{\sqrt{5}} \times \prod_{uv \in E_3} \frac{1}{\sqrt{6}} = \left(\frac{1}{5}\right)^{2sR} \times \left(\frac{1}{\sqrt{6}}\right)^{(6R+3)st-5sR}$$

Inference 5

Nanostructure	V-Phenylenic	V-Naphatalenic	V-Anthracene	V-Tetracenic
$XII(H)$	$\left(\frac{1}{5}\right)^{2s} \times \left(\frac{1}{\sqrt{6}}\right)^{9st-5s}$	$\left(\frac{1}{5}\right)^{4s} \times \left(\frac{1}{\sqrt{6}}\right)^{15st-10s}$	$\left(\frac{1}{5}\right)^{6s} \times \left(\frac{1}{\sqrt{6}}\right)^{21st-15s}$	$\left(\frac{1}{5}\right)^{8s} \times \left(\frac{1}{\sqrt{6}}\right)^{27st-20s}$

$$(6). \quad \chi II(H) = \prod_{uv \in E(H)} \frac{1}{\sqrt{d_H(u)d_H(v)}} = \left(\frac{1}{\sqrt{6}}\right)^{4sR} \times \left(\frac{1}{\sqrt{9}}\right)^{(6R+3)st-5sR}$$

$$= \prod_{uv \in E_2} \frac{1}{\sqrt{6}} \times \prod_{uv \in E_3} \frac{1}{\sqrt{9}} = 2^{-2sR} \times 3^{3sR-(6R+3)st}$$

Inference 6

Nanostructure	V-Phenylenic	V-Naphatalenic	V-Anthracene	V-Tetracenic
$\chi II(H)$	$2^{-2s} \times 3^{3s-9st}$	$2^{-4s} \times 3^{6s-15st}$	$2^{-6s} \times 3^{9s-21st}$	$2^{-8s} \times 3^{12s-27st}$

$$(7). \quad MZ_1^a(H) = \prod_{uv \in E(H)} [d_H(u) + d_H(v)]^a = 5^{a(4sR)} \times 6^{a[(6R+3)st-5sR]}$$

$$= \prod_{uv \in E_2} 5^a \times \prod_{uv \in E_3} 6^a = 5^{4sRa} \times 6^{(6R+3)sta-5sRa}$$

Inference 7

Nanostructure	V-Phenylenic	V-Naphatalenic	V-Anthracene	V-Tetracenic
$MZ_1^a(H)$	$5^{4sa} \times 6^{9sta-5sa}$	$5^{8sa} \times 6^{15sta-10sa}$	$5^{12sa} \times 6^{21sta-15sa}$	$5^{16sa} \times 6^{27sta-20sa}$

$$\begin{aligned}
 (8). \quad MZ_2^a(H) &= \prod_{uv \in E(H)} [d_H(u)d_H(v)]^a &&= 6^{a(4sR)} \times 9^{[a(6R+3)st-5sR]} \\
 &= \prod_{uv \in E_2} 6^a \times \prod_{uv \in E_3} 9^a &&= 2^{4sRa} \times 3^{(6R+3)2sta-6sRa}
 \end{aligned}$$

Inference 8

Nanostructure	V-Phenylenic	V-Naphatalenic	V-Anthracene	V-Tetracenic
$MZ_2^a(H)$	$2^{4sa} \times 3^{18sta-6sa}$	$2^{8sa} \times 3^{30sta-12sa}$	$2^{12sa} \times 3^{42sta-18sa}$	$2^{16sa} \times 3^{54sta-24sa} \oplus$

$$\begin{aligned}
 (9). \quad ABCII(H) &= \prod_{uv \in E(H)} \sqrt{\frac{d_H(u) + d_H(v) - 2}{d_H(u)d_H(v)}} &&= \left(\frac{1}{\sqrt{2}}\right)^{4sT} \times \left(\frac{2}{3}\right)^{(6R+3)st-5sR} \\
 &= \prod_{uv \in E_2} \sqrt{\frac{3+2-2}{3 \times 2}} \times \prod_{uv \in E_3} \sqrt{\frac{3+3-2}{3 \times 3}} &&= 2^{(6R+3)st-7sR} \times 3^{5sR-(6R+3)st}
 \end{aligned}$$

Inference 9

Nanostructure	V-Phenylenic	V-Naphatalenic	V-Anthracene	V-Tetracenic
$ABCII(H)$	$2^{9st-7s} \times 3^{5s-9st}$	$2^{15st-14s} \times 3^{10s-15st}$	$2^{21st-21s} \times 3^{5s-21st}$	$2^{27st-28s} \times 3^{20s-27st}$

$$\begin{aligned}
 (10). \quad GAI(H) &= \prod_{uv \in E(H)} \frac{2\sqrt{d_H(u)d_H(v)}}{d_H(u) + d_H(v)} &&= \left(\frac{2\sqrt{6}}{5}\right)^{4sR} \times (1)^{(6R+3)st-5sR} \\
 &= \prod_{uv \in E_2} \frac{2\sqrt{3 \times 2}}{3+2} \times \prod_{uv \in E_3} \frac{2\sqrt{3 \times 3}}{3+3} &&= \left(\frac{2\sqrt{6}}{5}\right)^{4sR}
 \end{aligned}$$

Inference 10

Nanostructure	V-Phenylenic	V-Naphatalenic	V-Anthracene	V-Tetracenic
$GAI(H)$	$\left(\frac{2\sqrt{6}}{5}\right)^{4s}$	$\left(\frac{2\sqrt{6}}{5}\right)^{8s}$	$\left(\frac{2\sqrt{6}}{5}\right)^{12s}$	$\left(\frac{2\sqrt{6}}{5}\right)^{16s}$

$$\begin{aligned}
 (11). \quad GA^a II(H) &= \prod_{uv \in E(H)} \left(\frac{2\sqrt{d_H(u)d_H(v)}}{d_H(u) + d_H(v)}\right)^a &&= \left(\frac{2\sqrt{6}}{5}\right)^{4saR} \times (1)^{[a(6R+3)st-5sR]} \\
 &= \prod_{uv \in E_2} \left(\frac{2\sqrt{3 \times 2}}{3+2}\right)^a \times \prod_{uv \in E_3} \left(\frac{2\sqrt{3 \times 3}}{3+3}\right)^a &&= \left(\frac{2\sqrt{6}}{5}\right)^{4saR}
 \end{aligned}$$

Inference 11

Nanostructure	V-Phenylenic	V-Naphatalenic	V-Anthracene	V-Tetracenic
$GA^a II(H)$	$\left(\frac{2\sqrt{6}}{5}\right)^{4sa}$	$\left(\frac{2\sqrt{6}}{5}\right)^{8sa}$	$\left(\frac{2\sqrt{6}}{5}\right)^{12sa}$	$\left(\frac{2\sqrt{6}}{5}\right)^{16sa}$

Conclusion

In this article, we have studied the Multiplicative indices of some nanostructures. The analytical expression for the topological invariants is presented by using edge set dividing method. Also, we expressed the generalized form for the computational formulas. These proposed results will be useful for the study of nanostructures. The results obtained in this study have a wide application prospect in nanoscience, biology, pharmacy and other fields.

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