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Two Types of Geometric–Arithmetic index of V–phenylenic Nanotube

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ABSTRACT

The concept of geometric-arithmetic indices was introduced in the chemical graph theory. These indices are defined by the following general formula:

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{Q_u Q_v}}{Q_u + Q_v},$$

where Q_u is some quantity that in a unique manner can be associated with the vertex u of graph G. In this paper the exact formula for two types of geometric-arithmetic index of V-phenylenic nanotube are given.

Keywords: GA index, V–phenylenic nanotube.

1. INTRODUCTION

Throughout this section G is a simple connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. A topological index is a numeric quantity from the structure of a graph which is invariant under automorphisms of the graph under consideration.

A topological index is a numeric quantity from the structural graph of a molecule. Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of types of alkanes known as paraffin. The concept of geometric-arithmetic indices was introduced in the chemical graph theory. These indices

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generally are defined as $GA_{general} = GA_{general}(G) = \sum_{uv \in E(G)} \frac{2\sqrt{Q_u Q_v}}{Q_u + Q_v}$, where Q_u is some quantity that in a unique manner can be associated with the vertex *u* of graph *G*. The first type of geometric-arithmetic index is denoted by GA_1 and defined as $GA_1 = GA_1(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$, where *uv* is an edge of the molecular graph *G* and d_u stand for the degree of the vertex *u,* see [1].

The second type of geometric-arithmetic index is denoted by GA_2 and defined as $GA_2 = GA_2(G) = \sum_{uv \in E(G)} \frac{2\sqrt{n_u n_v}}{n_u + n_v}$, where n_u is the number of vertices of *G* lying closer to *u* than to *v* and n_v is the number of vertices of *G* lying closer to *v* than to *u*, see [2]. For $uv \in E(G)$, let m_u is the number of edges of *G* lying closer to *u* than to *v* and m_v is the number of edges of *G* lying closer to *v* than to *u*.

The third member of the class of $GA_{general}$ by setting Q_u (Q_v) to be the number m_u (m_v) for the edge *uv* of the graph *G* is defined as $GA_3 = GA_3(G) = \sum_{uv \in E(G)} \frac{2\sqrt{m_u m_v}}{m_u + m_v}$, it has been introduced in the paper [3]. A *V-phenylenic* net is a trivalent decoration made by alternating squares C_4 and hexagons C_6 and octagons C_8. In recent years, some researchers are interested to topological indices of *V-phenylenic* nanotube see [4] for details.

Throughout this paper *VU*= *VU* [*p*, *q*] denotes an arbitrary *V-phenylenic* nanotube in terms of the number of hexagons in a fixed row (*p*) and the number of hexagons in a fixed column (*q*), Figure 1.

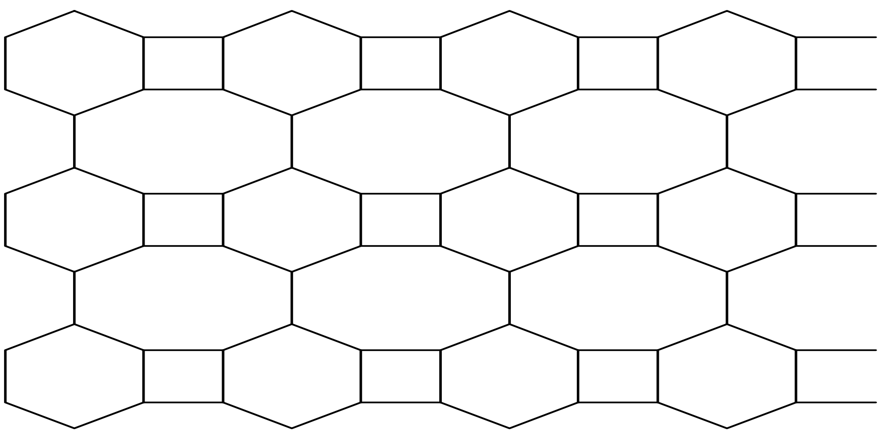

Figure 1. *V-phenylenic* Nanotube, with *p=4* and *q=3.*

2 MAIN RESULTS

In this section, GA_2 index of the molecular graph of *V-phenylenic* nanotube is computed. It is easy to see that

$$|V(VU)|=|V(VU[p,q])|=6pq \quad \text{and} \quad |E(VU)|=|E(VU[p,q])|=9pq-p.$$

In the following theorem the GA_2 index of *V-phenylenic* nanotube is obtained.

Theorem 1. The GA_2 index of *VU=VU* [*p, q*] is computed as follows:

$$GA_2(VU)=2pq+\sum_{uv\in E_2(T)}\frac{2\sqrt{n_u n_v}}{n_u+n_v}+\frac{4p}{3pq-p}$$
$$+\frac{4p}{pq-p}\sum_{k=1,k \text{ is odd}}^{q}\sqrt{(3pk)(|V(VU)|-3pk)}+\frac{2p}{3pq-p}\sum_{k=1,k \text{ is even}}^{q}\sqrt{(3pk)(|V(VU)|-3pk)}$$

Proof. One can see that there are three separate types of edges of *V-phenylenic* nanotube and the number of edges is different. Suppose e_1, e_2 and e_3 are representative edges for these types.

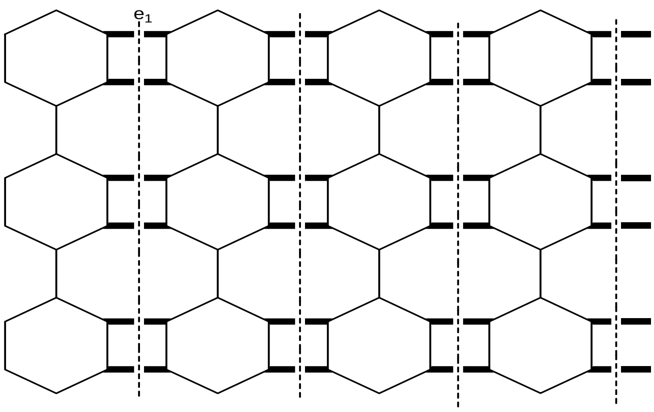

Figure 2. The Set $E_1(VU)$ (The Edges of Type e_1).

We partition the edges of *V-phenylenic* nanotube into three subsets $E_1(VU)$, $E_2(VU)$ and $E_3(VU)$, as follows:

$E_1(VU)$ = { e| e is the type of e_1},
$E_2(VU)$ = { e| e is the type of $e_{2,k}$ for $1\le k\le 2q$ },
$E_3(VU)$ = { e| e is the type of e_3}.

The sets $E_1(VU)$, $E_2(VU)$ and $E_3(VU)$ are shown by dashed lines in Figures 2, 3 and 4, respectively.

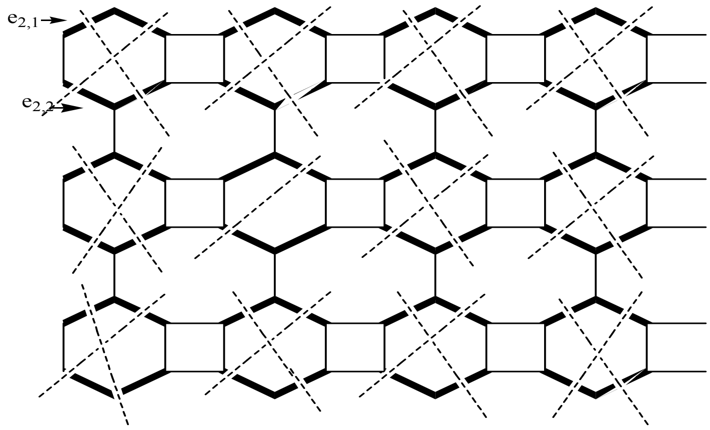

Figure 3. The Set $E_2(VU)$ (The Edges of Type e_2).

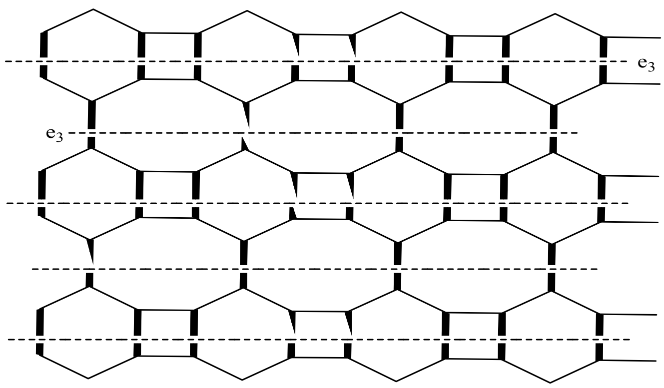

Figure 4. The Set $E_3(VU)$ (The Edges of Type e_3).

Therefore, by definition of GA_2 index,

$$GA_2(T) = \sum_{uv\in E_1(VU)} \frac{2\sqrt{n_u n_v}}{n_u + n_v} + \sum_{uv\in E_2(VU)} \frac{2\sqrt{n_u n_v}}{n_u + n_v} + \sum_{uv\in E_3(VU)} \frac{2\sqrt{n_u n_v}}{n_u + n_v} .$$

We evaluate each summation separately. For evaluating the first sum, we know that for $e = uv \in E_1(VU)$, if p is even we have $n_u = n_v = \frac{|V(VU)|}{2}$, if p is odd $n_u = n_v = \frac{|V(VU) - 2q|}{2}$ Also $|E_1(VU)| = 2pq$, then

$$\sum_{uv\in E(VU)_1}\frac{2\sqrt{n_u n_v}}{n_u+n_v}=2pq.$$

For each $e=uv\in E_2(VU)$, we have $n_u+n_v=4pq$. Suppose i is an odd positive integer, such that $1\le i\le q$,if p is even, we have

$$n_V(e)=\begin{cases}3pi-p & p<2q-i+1 \quad ,2p<i\\ \frac{3}{4}(p+i)^2-\frac{3}{4} & p<2q-i+1 \quad ,2p\ge i\\ 3pq-3q^2+3iq-q & p\ge 2q-i+1\end{cases}.$$

Suppose i is an even positive integer, such that $1\le i\le q$, if p is odd, we have

$$n_V(e)=\begin{cases}3pi-2p & p<2q-i+1,\ p<i\\ \frac{1}{4}(3p^2+6pi-4p+3i^2-4i) & p<2q-i+1,\ p\ge i\\ 3pq-3q^2+3qi-2q & p\ge 2q-i+1\end{cases}.$$

Suppose i is an even positive integer, such that $1\le i\le q$

$$n_V(e)=\begin{cases}6pq-3pi+p & p\le i, p \text{ is odd}\\ 6pq-3pi+2p & p\le i, p \text{ is even}\\ 3pq+\frac{1}{4}(-3p^2+6pi+14p-12qi+9i^2+2i+12q-11) & p>i,\ q>\frac{p+i-1}{2},\ p \text{ is odd}\\ 3pq-3q^2+3qi+7q & p>i, q\le\frac{p+i-1}{2}, p \text{ is odd}\\ 3pq-3q^2+3qi+2q & p>i,\ p \text{ is even}\end{cases}.$$

For all case, if p is odd, we have

$$n_u(e)=\begin{cases}|V(T)|-n_v-p-\left[\frac{i+1}{2}\right] & p<2q-i-1,\ p\neq 1\\ 2 & p=1\\ |V(T)|-n_v-2q & p\geq 2q-i-1\end{cases}.$$

If p is even, we have $n_u=|V(T)|-n_v$. Finally for computing the third sum, we attend, for each $e=uv\in E_3(VU)$ in i-th row, $n_u=3pi$ and $n_v=6pq-3pi$ and the number of edges of third type in each row is $2p$. Since *V*phenylenic nanotube is bipartite then for each $e=uv\in E_3(VU)$, we have $n_u+n_v=|V(VU)|$. Then

$$\sum_{uv\in E_3(VU)}\frac{2\sqrt{n_un_v}}{n_u+n_v}=\frac{2}{}\sum_{uv\in E_3(VU)}\sqrt{n_un_v}=\frac{4p}{6pq}\sum_{k=1,k\text{ is odd}}^{q}\sqrt{(3pk)(|V(T)|-3pk)}$$
$$+\frac{2p}{6pq}\sum_{k=2,k\text{ is even}}^{q}\sqrt{(3pk)(|V(T)|-3pk)}$$
$$=\frac{2}{3q}\sum_{k=1,k\text{ is odd}}^{2q-1}\sqrt{(3pk)(|V(T)|-3pk)}$$
$$+\frac{1}{3q}\sum_{k=1,k\text{ is even}}^{q}\sqrt{(3pk)(|V(T)|-3pk)}.$$

Theorem 2. The GA_3 index of $VU=VU[p,q]$ is given by:

$$GA3(VU)=2pq+\sum_{uv\in E_2(VU)}\frac{2\sqrt{m_um_v}}{m_u+m_v}+\frac{2p}{12pq-4p}\sum_{k=0}^{2q-2}\sqrt{(4p+6kp)(12pq-8p-6kp)},$$

where the elements of $E_2(VU)$ are shown in Figure 4.

Proof. The sets of $E_1(VU)$, $E_2(VU)$ and $E_3(VU)$, are defined in the same way as is the previous theorem. Therefore, by definition of GA_3 index,

$$GA_3(VU[p,q])=\sum_{uv\in E_1(VU)}\frac{2\sqrt{m_um_v}}{m_u+m_v}+\sum_{uv\in E_2(VU)}\frac{2\sqrt{m_um_v}}{m_u+m_v}+\sum_{uv\in E_3(VU)}\frac{2\sqrt{m_um_v}}{m_u+m_v}.$$

For each $e=uv\in E_1(VU)$, if p is even, we have: $m_u=m_v=\frac{m-4q}{2}$ and if p is odd, we have: $m_u=m_v=\frac{m-2q}{2}$. Then $\sum_{uv\in E_1(VU)}\frac{2\sqrt{m_um_v}}{m_u+m_v}=2pq$. We can partition E_2 (*VU*) into $2q$ subsets such as $E_{2,1}$, $E_{2,2}$, …, $E_{2,2q}$, such that $E_{2,k}=\{\,e|\ e$ is the type of $e_{2,k}\,\}$, for $1\leq k\leq 2q$. Therefore

$$\sum_{uv\in E_2(VU)}\frac{2\sqrt{m_u m_v}}{m_u+m_v}=2\sum_{k=1}^{q}\sum_{uv\in E_{2,i}}\frac{2\sqrt{m_u m_v}}{m_u+m_v}.$$

Suppose i is an odd positive integer and $2p \geq i$, such that $1 \leq i \leq q$, for each $e = uv \in E_{2,i}$. By calculation, we have the following results:

$$m_v(e)=\begin{cases}\frac{3}{4}(p+i-1)^2+\frac{1}{4}(p+i-1)(p+i+1)+ & p<2q-2\left[\frac{i-1}{2}\right], p \text{ is even}\\ \frac{1}{8}(p+i-3)(p+i-1). & \\ 1+\frac{3}{4}(p+i-2)^2+2(p+i-2)+ & p<2q-2\left[\frac{i-1}{2}\right], p \text{ is odd}\\ \frac{1}{4}(p+i-2)(p+i)+\frac{1}{8}(p+i-2)(p+i). & \\ 3pq-3q^2+3(i-1)q+q(q+1)+ & p\geq 2q-2\left[\frac{i-1}{2}\right], p \text{ is even}\\ 2q\left(\frac{p-2q+i-1}{2}\right)+\frac{q(q+1)}{2}+(q-1)\left(\frac{p-2q+i-1}{2}\right). & \\ 3pq-3q^2+(3i-2)q+q(q+1)+ & p\geq 2q-2\left[\frac{i-1}{2}\right], p \text{ is odd}\\ 2q\left(\frac{p-2q+i-1}{2}\right)+\frac{q(q+1)}{2}+(q-1)(\frac{p-2q+i-2}{2}). & \end{cases}$$

$$m_u(e)=\begin{cases}|E(VU)|-m_v(e)-(2p+2i-2) & p<2q-2\left[\frac{i-1}{2}\right], p \text{ is even}\\ |E(VU)|-m_v(e)-(\frac{3}{2}p+3i-\frac{3}{2}) & p<2q-2\left[\frac{i-1}{2}\right], p \text{ is odd}\\ |E(VU)|-m_v(e)-4q & p\geq 2q-2\left[\frac{i-1}{2}\right], p \text{ is even}\\ |E(VU)|-m_v(e)-3q & p\geq 2q-2\left[\frac{i-1}{2}\right], p \text{ is odd}\end{cases}$$

Suppose i is an even positive integer and $2p \geq i$, such that $1 \leq i \leq q$, for each $e = uv \in E_{2,i}$,

$$m_V(e)=\begin{cases} \frac{3}{4}(p+i-2)^2+(p+i-2)+ & p<2q-2\left[\frac{i-1}{2}\right], \ p \text{ is even} \\ \frac{1}{4}(p+i-2)(p+i)+\frac{1}{8}(p+i-4)(p+i+2) & \\ \frac{3}{4}(p+i-1)^2+\frac{1}{4}(p+i-1)^2 & p<2q-2\left[\frac{i-1}{2}\right], \ p \text{ is odd} \\ +\frac{1}{8}(p+i-3)(p+i-1) & \\ 3pq-3q^2+(6i-4)q+q(q+1)+ & p\geq 2q-2\left[\frac{i-1}{2}\right], \ p \text{ is even} \\ 2q\left(\frac{p-2q+i-2}{2}\right)+\frac{q(q+1)}{2}-1+(q-1)\left(\frac{p-2q+i-2}{2}\right) & \\ 3pq-3q^2+(6i-3)q+q(q+2)+ & p\geq 2q-2\left[\frac{i-1}{2}\right], \ p \text{ is odd} \\ 2q\left(\frac{p-2q+i-3}{2}\right)+\frac{q(q+1)}{2}-1+(q-1)\left(\frac{p-2q+i-3}{2}\right) & \end{cases}$$

and

$$m_U(e)=\begin{cases} |E(VU)|-m_V(e)-(2p+2i-2) & p<2q-2\left[\frac{i-1}{2}\right], \ p \text{ is even} \\ |E(VU)|-m_V(e)-(\frac{3}{2}p+3i-\frac{3}{2}) & p<2q-2\left[\frac{i-1}{2}\right], \ p \text{ is odd} \\ |E(VU)|-m_V(e)-4q & p\geq 2q-2\left[\frac{i-1}{2}\right], \ p \text{ is even} \\ |E(VU)|-m_V(e)-3q & p\geq 2q-2\left[\frac{i-1}{2}\right], \ p \text{ is odd} \end{cases}$$

Suppose i is an odd positive integer and $2p<i$, such that $1\leq i\leq q$, for each $e=uv\in E_{2,i}$,

$$m_V(e)=\begin{cases} p\left(\frac{3p-1}{2}\right)+(p-1)\left(\frac{3p-2}{2}\right)+3p(i-p)+ip+\frac{p}{2}(i-1)+p\left(\frac{i-2p-1}{2}\right) & p \text{ is even} \\ 1+(p-1)(3p+1)+3p(i-p)+(i-1)p+p^2+p\left(\frac{i-2p-1}{2}\right) & p \text{ is odd} \end{cases}$$

and

$$m_u(e)=\begin{cases}|E(VU)|-m_v(e)-(4p-2) & p \text{ is even}\\ |E(VU)|-m_v(e)-(3p-1) & p \text{ is odd}\end{cases}$$

Suppose i is an even positive integer and $2p<i$, such that $1\le i\le q$, for each $e=uv\in E_{2,i}$,

$$m_v(e)=\begin{cases}p\left(\frac{3p-1}{2}\right)+(p-1)\left(\frac{3p-2}{2}\right)+3p(3q-p-2i+1) & p \text{ is even}\\ +p(i+1)+2p(q-i)+\frac{p}{2}(i-1)+p(q-i) & \\ 1+(p-1)(3p+1)+3p(3q-p-2i+1)+ & p \text{ is odd}\\ ip+2p(q-i)+p\left(\frac{i}{2}\right)+p(q-i) & \end{cases}$$

and

$$m_u(e)=\begin{cases}|E(VU)|-m_v(e)-(4p-2) & p \text{ is even}\\ |E(VU)|-m_v(e)-3p & p \text{ is odd}\end{cases} \quad \text{for } e=uv\in E3(UV)$$

For $e=uv\in E_3(VU)$

$$m_u(e)=m_u(e)=\begin{cases}\frac{m-p}{2} & \text{On octagon vertical edges}\\ \frac{m-2p}{2} & \text{On hexagon vertical edes}\end{cases}$$

Hence $\sum_{uv\in E_3(VU)}\frac{2\sqrt{m_u m_v}}{m_u+m_v}=2pq+q-1.$ This completes the proof. □

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