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Two Types of Geometric-Arithmetic Indices of Nanotubes and Nanotori

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Abstract

The concept of geometric-arithmetic indices was introduced in the chemical graph theory. These indices are defined as $GA(G) = \sum_{uv\in E(G)} 2\sqrt{Q_u \cdot Q_v}/(Q_u + Q_v)$, where Q_u is some quantity that in a unique manner can be associated with the vertex *u* of graph *G*. In this paper, exact formulas for two types of geometric-arithmetic index of $TUC_4C_8(S)$ nanotube and $TC_4C_8(S)$ nanotorus are given.

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 Wiener index of *G* is the sum of distance between all unordered pair of vertices of *G*, $W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v)$, where $d_G(u,v)$ and is defined as the number of edges in a minimal path connecting the vertices *u* and *v,* see [1]. The concept of geometric-arithmetic indices was introduced in the chemical graph theory. These indices generally are defined as

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

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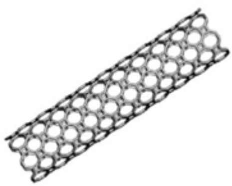
where Q_u is some quantity that in a unique manner can be associated with the vertex u of graph G.

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 [2]. The GA_1 index has been introduced less than a year ago [2]. However, a few papers are appeared dealing with this quantity, see [3-5].

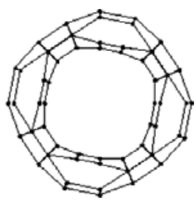
The second type of geometric-arithmetic index is denoted by GA_2 and defined as $GA_2 = GA_2(G) = \sum_{uv\in E(G)} \frac{2\sqrt{n_u n_v}}{n_u + n_v}$, where n_u is the number of vertices of G lying closer to u than to v and n_v is the number of vertices of G lying closer to v than to u, see [6]. For $uv \in E(G)$, 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 [7]. A C_4C_8 net is a trivalent decoration made by alternating squares C_4 and octagons C_8. In recent years, some researchers are interested to topological indices of C_4C_8 nanotubes and nanotori, see [8-21] for details. They computed some distance based topological indices of these nanotubes and nanotori.

The $TUC_4C_8(S)$ nanotube is a mathematically beautiful object constructed from squares and octagons, Figure 1 (a). The aim of this article is to compute GA_2 and GA_3 indices of $TUC_4C_8(S)$ nanotube and $TC_4C_8(S)$ nanotorus that obtained from $TUC_4C_8(S)$ nanotube by gluing its ends, Figure 1 (b).



a



b

Figure 1. (a) $TUC_4C_8(S)$ nanotube, (b) $TC_4C_8(S)$ nanotorus.

Throughout this paper $T= T[p, q]$ denotes an arbitrary $TUC_4C_8(S)$ nanotube in terms of the number of octagons in a fixed row (p) and the number of octagons in a fixed column (q), in the two-dimensional lattice of T , Figure 2. We also denote a $TC_4C_8(S)$ nanotorus, Figure 3, by $S= S[p, q]$.

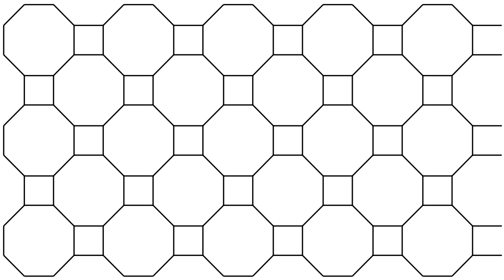


Figure 2. Two Dimensional Lattice $TUC_4C_8(S)$ nanotube, with $p=5$ and $q=3$.

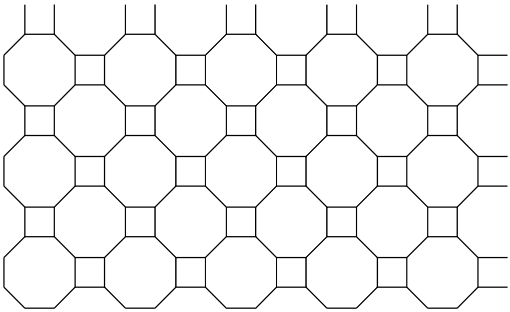


Figure 3. Two Dimensional Lattice $TC_4C_8(S)$ nanotorus, with $p=5$ and $q=3$.

2. Main Results

In this section, GA_2 and GA_3 indices of the molecular graph of $TUC_4C_8(S)$ nanotube and $TC_4C_8(S)$ nanotorus are computed. It is easy to see that

$$|V(T)|=|V(T[p,q])|=8pq \text{ and } |E(T)|=|E(T[p,q])|=12pq-2p,$$

$$|V(S)|=|V(S[p,q])|=8pq \text{ and } |E(S)|=|E(S[p,q])|=12pq.$$

In the following theorem the GA_2 index of $TUC_4C_8(S)$ nanotube is obtained.

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

$$GA_2(T)=\begin{cases} 4pq+\dfrac{1}{4pq}\sum_{k=1}^{p}\sqrt{(p+k-1)(p+k)\big(|V(T)|-(p+k-1)(p+k)\big)} \\ \qquad +\dfrac{1}{2q}\sum_{k=1}^{2q-1}\sqrt{4pk(|V(T)|-4pk)} & p\le\dfrac{q}{2} \\ 4pq+\dfrac{1}{4pq}\sum_{k=1}^{p}\sqrt{(4q^2+2q-4kq)\big(|V(T)|-(4q^2+2q-4kq)\big)} & p>\dfrac{q}{2} \\ \qquad +\dfrac{1}{2q}\sum_{k=1}^{2q-1}\sqrt{4pk(|V(T)|-4pk)} \end{cases}.$$

Proof. One can see that there are three separate types of edges of $TUC_4C_8(S)$ nanotube and the number of edges is different. Suppose e_1, e_2 and e_3 are representative edges for these types.

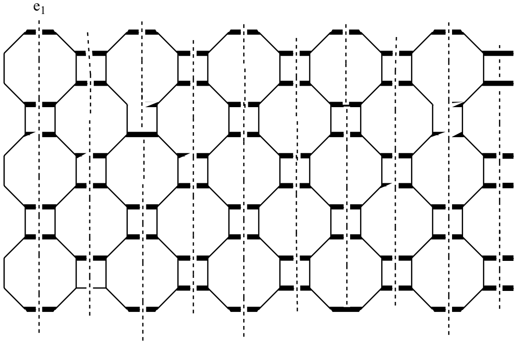


Figure 4. The set $E_1(T)$ (The edges of type e_1).

We partition the edges of $TUC_4C_8(S)$ nanotube into three subsets $E_1(T)$, $E_2(T)$ and $E_3(T)$, as follows:

$E_1(T)$= { e| e is the type of e_1},

$E_2(T)$= { e| e is the type of $e_{2,k}$ for $1\le k\le 2q$ },

$E_3(T)$= { e| e is the type of e_3}.

The sets $E_1(T)$, $E_2(T)$ and $E_3(T)$ are shown by dashed lines in Figures 4, 5 and 6, respectively.

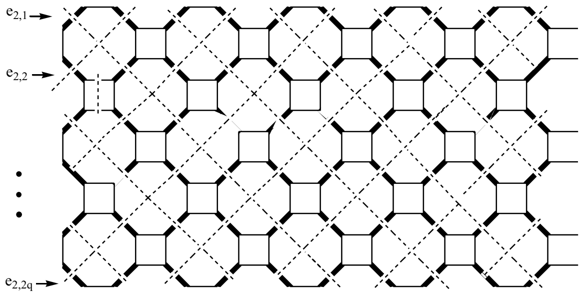


Figure 5. The set $E_2(T)$ (The edges of type e_2).

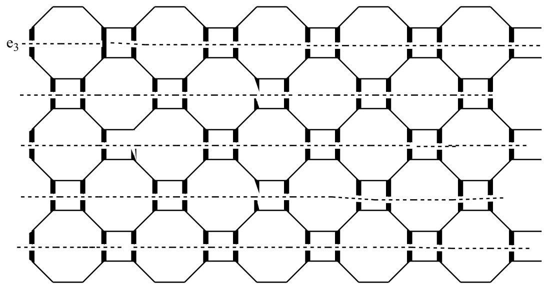


Figure 6. The set $E_3(T)$ (The edges of type e_3).

Therefore, by definition of GA_2 index,

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

We evaluate each sums separately. For evaluating the first sum, we know that for $e=uv\in E_1(T)$, we have $n_u=n_v=\frac{|V(T)|}{2}$. Also $|E_1(T)|=4pq$, then $\sum_{uv\in E(T)_1}\frac{2\sqrt{n_un_v}}{n_u+n_v}=4pq$.

For each $e=uv\in E_2(T)$, we have $n_u+n_v=8pq$. Obviously, for every $e_{2,1}=uv$, we have $n_u=p(p+1), n_v=8pq-p(p+1)$, for every $e_{2,2}=uv$, we have $n_u=(p+1)(p+2), n_v=8pq-(p+1)(p+2)$, …, for every $e_{2,i}=uv$, we have

$n_u=(p+i-1)(p+i), n_v=8pq-(p+i-1)(p+i)$ .So

$$\sum_{uv\in E_2(T)}\frac{2\sqrt{n_u n_v}}{n_u+n_v}=\frac{1}{4pq}\sum_{i=1}^{q}\sqrt{(p+i-1)(p+i)[8pq-(p+i-1)(p+i)]}.$$

By the same method when $p>\frac{q}{2}$, we can compute $\sum_{uv\in E_2(T)}\frac{2\sqrt{n_u n_v}}{n_u+n_v}$.

Finally for computing the third sum, we attend, for each $e=uv\in E_3(T)$ in k-th row, n_u= $4pk$ and n_v= $8pq-4pk$ and the number of edges of third type in each row is $2p$. Since $TUC_4C_8(S)$ nanotube is bipartite then for each $e=uv\in E_3(T)$, we have $n_u+n_v=|V(T)|$. Then

$$\sum_{uv\in E_3(T)}\frac{2\sqrt{n_u n_v}}{n_u+n_v}=\frac{1}{4pq}\sum_{uv\in E_3(T)}\sqrt{n_u n_v}=\frac{2p}{4pq}\sum_{k=1}^{2q-1}\sqrt{(4pk)(|V(T)|-4pk)}$$
$$=\frac{1}{2q}\sum_{k=1}^{2q-1}\sqrt{(4pk)(|V(T)|-4pk)}.$$

This completes the proof. □

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

$$GA_3(T)=4pq+\sum_{uv\in E_2(T)}\frac{2\sqrt{m_u m_v}}{m_u+m_v}+\frac{2p}{12pq-4p}\sum_{k=0}^{2q-2}\sqrt{(4p+6kp)(12pq-8p-6kp)},$$

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

Proof. We can now state the analogue of Theorem 1. Then

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

For each $e=uv\in E_1(T)$, $m_u=m_v=\frac{m-2q}{2}$, then $\sum_{uv\in E_1(T)}\frac{2\sqrt{m_u m_v}}{m_u+m_v}=4pq$. We can partition $E_2(T)$ 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 $1\le k\le 2q$. Therefore

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

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

$$m_v(e)=\begin{cases}(p+i-1)^2+\left[\dfrac{p^2}{2}\right]+(i-1)p+\dfrac{(i-1)^2}{2} & p<2q-2\left[\dfrac{i-1}{2}\right]\\[2ex] 6pq-6q^2+(6i-4)q-2p+2\left[\dfrac{p}{2}\right]-i+1 & p\geq 2q-2\left[\dfrac{i-1}{2}\right]\end{cases}$$

and

$$m_u(e)=\begin{cases}|E(T)|-m_v(e)-(2p+2i-2) & p<2q-2\left[\dfrac{i-1}{2}\right]\\[2ex] |E(T)|-m_v(e)-4pq & p\geq 2q-2\left[\dfrac{i-1}{2}\right]\end{cases}.$$

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

$$m_v(e)=\begin{cases}(p+i-1)^2+\left[\dfrac{p^2+1}{2}\right]+(i-1)p+\dfrac{i}{2}(i-2) & p<2q-2\left[\dfrac{i-1}{2}\right]\\[2ex] 6pq-6q^2+(6i-4)q-2p-2\left[\dfrac{p}{2}\right]-i & p\geq 2q-2\left[\dfrac{i-1}{2}\right]\end{cases}$$

and

$$m_u(e)=\begin{cases}|E(T)|-m_v(e)-(2p+2i-2) & p<2q-2\left[\dfrac{i-1}{2}\right]\\[2ex] |E(T)|-m_v(e)-4pq & p\geq 2q-2\left[\dfrac{i-1}{2}\right]\end{cases}.$$

For $e=uv\in E_3(T)$, in k-th row, $m_u+m_v=12pq-4p$ and then, $m_u=4p+6pk$, $m_v=12pq-8p-6pk$. Hence $\sum_{uv\in E_3(T)}\frac{2\sqrt{m_u m_v}}{m_u+m_v}=\frac{2p}{12pq-4p}\sum_{k=0}^{2q-2}\sqrt{(4p+6pk)(12pq-8p-6pk)}$. This completes the proof. □

Theorem 3. The GA_2 and GA_3 indices of $S=S[p, q]$ are equal and computed as follows:

$$GA_2(S)=GA_3(S)=|E(S)|.$$

Proof. Since $TC_4C_8(S)$ nanotori is bipartite then for each $e=uv\in E(S)$, we have $n_u+n_v=|V(S)|$. Moreover for each $e=uv\in E(S)$, $n_u=n_v=\frac{|V(S)|}{2}$, therefore by definition of

GA_2 index we conclude that, $GA_2(S)=\sum_{uv\in E(S)}\frac{2\sqrt{n_u n_v}}{n_u+n_v}=|E(S)|$. Now for obtaining the GA_3 index, it is sufficient to show that for each $e=uv\in E(S)$, $m_u=m_v$. Such as Theorem 1, we partition the edge set of $S=S\,[p,\,q]$ into three subsets $E_1(S)$, $E_2(S)$ and $E_3(S)$, these subsets are shown in Figure 7 by dashed lines.

For each $e=uv\in E_1(S)$, $m_u=m_v=\frac{|E(S)|-2q}{2}$. For second type of edges for each $e=uv\in E_2(S)$, $m_u=m_v=\frac{|E(S)|-(10+6(r-2))}{2}=\frac{|E(S)|+2-6r}{2}$, where $r = min\{p,q\}$. Finally for each $e=uv\in E_3(S)$, $m_u=m_v=\frac{|E(S)|-2p}{2}$. By above argument, we conclude that

$$\begin{aligned}GA_3(S)&=\sum_{uv\in E_1(S)}\frac{2\sqrt{m_u m_v}}{m_u+m_v}+\sum_{uv\in E_2(S)}\frac{2\sqrt{m_u m_v}}{m_u+m_v}+\sum_{uv\in E_3(S)}\frac{2\sqrt{m_u m_v}}{m_u+m_v}\\&=|E_1(S)|+|E_2(S)|+|E_3(S)|=|E(S)|,\end{aligned}$$

and this complete the proof. □

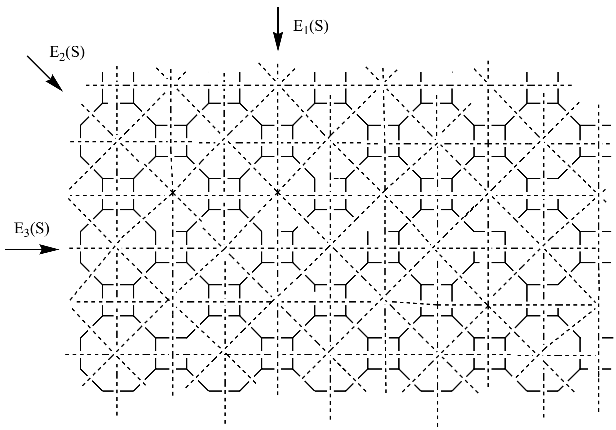


Figure 7. The partition of E(S) into $E_1(S)$, $E_2(S)$ and $E_3(S)$.

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