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On the Edge and Total GA Indices of Nanotubes

[1]*Anehgaldi Mahmiani and* [2]*Omid Khormali*

[1]Department of Mathematics, Payame Noor University, 19395-4697 Tehran, Iran
[2]Mathematics and Informatics Research Group, ACECR,
Tarbiat Modares University, P.O. Box: 14115-343, Tehran, Iran

Abstract: The total version of geometric–arithmetic (GA) index of graphs is introduced based on the end-vertex degrees of edges of their total graphs. In this paper, the total GA index is computed for zigzag polyhex nanotubes by using some results on GA index and mentioned nanotubes. Also, we compute the edge GA index for the subdivision graphs of $TUC_4C_8(R)$ and $TUAC_6$[p',q'] nanotubes.

Key words: Geometric–arithmetic index · Line graph · Total Graph · Degree (of a vertex) · Nanotubes

INTRODUCTION

A single number that can be used to characterize some property of the graph of a molecule is called a topological index for that graph. There are numerous topological descriptors that have found some applications in theoretical chemistry, especially in QSPR/QSAR research [1]. The oldest topological index which introduced by Harold Wiener in 1947 is ordinary (vertex) version of Wiener index [2] which is the sum of all distances between vertices of a graph. Also, the edge versions of Wiener index which were based on distance between edges introduced by Iranmanesh *et al*. 2008 [3].

One of the most important topological indices is the well-known branching index introduced by Randic [4] which is defined as the sum of certain bond contributions calculated from the vertex degree of the hydrogen suppressed molecular graphs.

Motivated by the definition of Randic connectivity index based on the end-vertex degrees of edges in a graph connected G with the vertex set $V(G)$ and the edge set $E(G)$ [5, 6], Vukicevic and Furtula [7] proposed a topological index named the geometric-arithmetic index (shortly GA) as:

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$$

where $d_G(u)$ denotes the degree of the vertex u in G. The reader can find more information about geometric-arithmetic index in [7-9].

It has been reported in the literature [10], the edge version of geometric-arithmetic index introduced based on the end-vertex degrees of edges in a line graph of G which is a graph such that each vertex of $L(G)$ represents an edge of G; and two vertices of $L(G)$ are adjacent if and only if their corresponding edges share a common endpoint in G, as follows:

$$GA_e(G) = \sum_{ef \in E(L(G))} \frac{2\sqrt{d_{L(G)}(e)d_{L(G)}(f)}}{d_{L(G)}(e)+d_{L(G)}(f)}$$

where $d_{L(G)}$ denotes the degree of the edge x in G.

The total version of geometric-arithmetic index is introduced based on the end-vertex degrees of edges in a total graph of G which is a graph such that the vertex set of $T(G)$ corresponds to the vertices and edges of G and two vertices are adjacent in $T(G)$ if and only if their corresponding elements are either adjacent or incident in G as follows:

$$GA_t(G) = \sum_{xy \in E(T(G))} \frac{2\sqrt{d_{T(G)}(x)d_{T(G)}(y)}}{d_{T(G)}(x)+d_{T(G)}(y)}$$

where $d_{T(G)}(x)$ denotes the degree of the vertex x in *T(G),* [12].

Corresponding Author: Omid Khormali, Mathematics and Informatics Research Group, ACECR, Tarbiat Modares University, P.O. Box: 14115-343, Tehran, Iran.

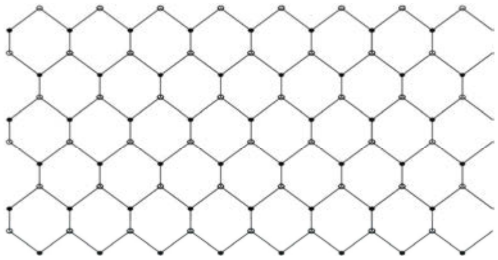

Fig. 1: Two dimensional lattice of zigzag polyhex nanotube, $q = 6$, $p = 8$

In next section, the total GA index is computed for graph of zigzag polyhex nanotubes.

The Total GA Index for Zigzag Polyhex Nanotubes: We use the notations q and p for the number of rows and number of hexagons in a row, respectively in the zigzag polyhex nanotubes which is mentioned in Figure 1 with $q = 6$ and $p = 8$. We denote zigzag polyhex nanotube with $Z(p,q)$.

In following we mention to two lemmas which we need in our computations.

Lemma 2.1: [13] Let G be a graph, $u \in V(G)$ and $e = vz \in E(G)$. Then we have:

$$d_{L(G)}(e) = d_G(v) + d_G(z) - 2$$

Lemma 2.2: [12] Let G be a graph, $u \in V(G)$ and $e = vz \in E(G)$. Then we have:

$$d_{T(G)}(e) = d_{L(G)}(e) + 2 = d_G(v) + d_G(z) \text{ and } d_{T(G)}(u) = 2d_G(u)$$

Now, we are ready to state the total GA index of zigzag polyhex nanotubes.

Theorem 2.3: The total GA index of zigzag polyhex nanotube is.

$$GA_t(Z(p,q)) = p(15q + \frac{16\sqrt{30}}{11} + \frac{16\sqrt{5}}{9} + \frac{8\sqrt{6}}{5} - 17)$$

Proof: Consider the zigzag polyhex nanotube. The number of edges of graph $Z(p,q)$, line graph $L(Z(p,q))$ and total graph $T(Z(p,q)$ are $3pq - p$, $6pq + 2p$ and $15pq - p$, respectively. If we consider to the edges of $Z(p,q)$ in $T(Z(p,q))$, there exist $4p$ edges with endpoints which have degrees 4 and 6 and $pq - 5p$ edges with endpoints which have degree 6.

If we consider to the edges of $L(Z(p,q))$ in $T(Z(p,q))$, there exist $4p$ edges with endpoints which have degrees 5 and 6, $4p$ edges with endpoints which have degrees 5 and 5 and $6pq - 6p$ edges with endpoints which have degree 6.

If we consider to the edges of $T(Z(p,q))$ that are not the edges of $Z(p,q)$ and $L(Z(p,q))$, there exist $4p$ edges with endpoints which have degrees 4 and 5, $4p$ edges with endpoints which have degrees 5 and 6 and $6pq - 10p$ edges with endpoints which have degree 6. Therefore, the desire result can be obtained.

In next section, we compute the edge GA index for the subdivision graphs of $TUC_4\,C_8\,(R)$ and $TUAC_6[p',q']$ nanotubes.

Edge GA Index for Two Subdivision Graphs: Firstly, we restate the subdivision graph which constructed from a graph G.

Suppose $G = (V, E)$ is a connected graph with the vertex set $V(G)$ and the edge set $E(G)$. Give a n edge $e = (u, v)$, let $V(e) = \{u, v\}$. The subdivision graph $S(G)$ which is related graphs to graph G have been defined as follows ([11]):

Subdivision Graph: $S(G)$ is the graph obtained from G by replacing each of its edge by a path of length two, or equivalently, by inserting an additional vertex into each edge of G. Figure 2(c).

Given $G = (V,E)$,

where $|E(G)| \subset \binom{V(G)}{2}$, we may define another set that we use:

$$EV(G) := \{\{e,v\}|\ e \in E(G), V(G) \ni v \in V(e)\}$$

We can write the subdivision operator above as follows:

$$S(G) := (V(G) \cup E(G), EV(G))$$

Now, we mention to $TUC_4C_8(R)$ and $TUAC_6[p',q']$ nanotubes.

We use the notations q and p for the number of rows of squares and number of squares in a row, respectively in the $TUC_4C_8(R)$ nanotubes which is mentioned in Figure 3 with $q = 4$ and $p = 8$. We denote $TUC_4C_8(R)$ nanotube with $T(p,q)$.

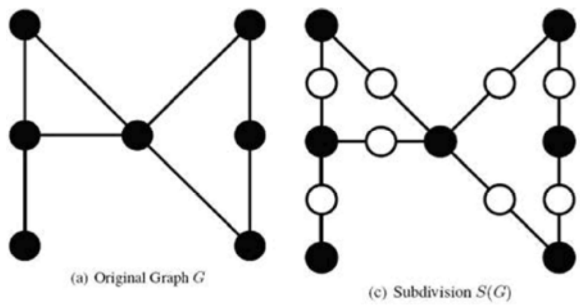

Fig. 2: The subdivision operator S(G)

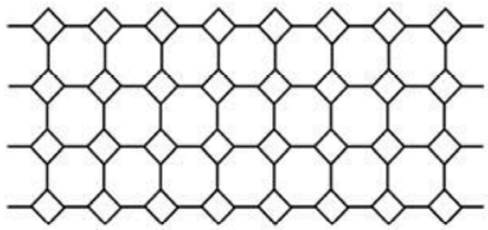

Fig. 3: Two dimensional lattice of $TUC_4C_8(R)$ nanotube, $q = 4$, $p = 8$

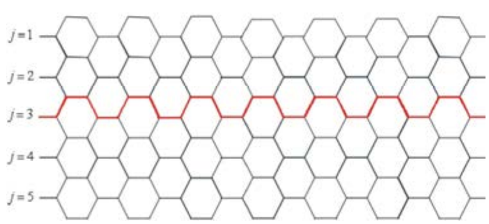

Fig. 4: Armchair polyhex nanotube, $TUAC_6[7,5]$, with $1 \le j \le 5$ rows

A single-wall carbon nanotube can be imagined as graphene sheet rolled at a certain "chiral" angle with respect to a plane perpendicular to the tube's long axis. Tubes having chiral angle = 30° are called "armchair". Armchair polyhex nanotube graph, that denoted by $TUAC_6$ $[p',q']$, is a nanotube that p' and q' are the number of hexagons in length and width of molecular graph, respectively. Also, it has j rows which $1 \le j \le q'$ as shown in Figure 4. In addition we denote $TUAC_6$ [p',q'] nanotube with T'(p',q'). Also, due to these notations, $|E(T'(p', q'))| = 6p'q' + p'$.

In the following we mention to two theorems from [13].

Theorem 3.1: [13] Let G be a graph with n vertices and m edges. Then we have:

$$GA(S(G)) = 2\sqrt{2} \sum_{u \in V(G)} \frac{(d_G(u))^{\frac{3}{2}}}{2 + d_G(u)}$$

Theorem 3.2: [13] Let G be a graph with n vertices and m edges. Then we have:

$$GA_e(S(G)) = \sum_{u \in V(G)} \binom{d_G(u)}{2} + GA(G)$$

Now, we ready to compute the edge GA index for subdivision graph of $TUC_4C_8(R)$ and $TUAC_6$[p',q'] nanotubes.

Theorem 3.3: The edge GA index for subdivision graphs of $TUC_4C_8(R)$ and $TUAC_6$[p',q'] nanotubes is:

$$GA_e(S(T(p,q))) = p\left(18q + \frac{4\sqrt{6}}{5} - 7\right)$$

$$GA_e(S(T'(p',q'))) = p'\left(18q' + \frac{8\sqrt{6}}{5} - 5\right)$$

Proof: Since the number of vertices of $TUC_4C_8(R)$ and $TUAC_6$[p',q'] nanotubes are $4pq$ and $4p'q' + 2p'$, we can compute easily by using Theorems 2.2 and 3.2 and following results.

$$GA(T(p,q)) = p\left(6q + \frac{4\sqrt{6}}{5} - 3\right) \text{ and}$$

$$GA(T'(p',q')) = p'\left(6q' + \frac{8\sqrt{6}}{5} - 3\right)$$

CONCLUSION

By using some results on different versions of GA index and also zigzag nanotubes, we compute the total GA index for zigzag polyhex nanotubes. Beside of this computation, the edge GA index for the subdivision graphs of $TUC_4C_8(R)$ and TUAC6[p',q'] nanotubes is computed.

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