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Computing the GA index of nanotubes and nanotori

H. SHABANI, A. R. ASHRAFI*
Department of Mathematics, Statistics and Computer Science, Faculty of Science, Kashan 87317-51167, I. R. Iran
Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, I. R. Iran

The *GA* index of a molecular graph *G* is defined as the sum of all $\frac{2\sqrt{deg(u)deg(v)}}{deg(u)+deg(v)}$ over all edges $e = uv$ of *G*, where $deg(u)$ denotes the degree of vertex *u* in *G*. In this paper the *GA* index of some nanotubes and nanotori are computed.

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1. Introduction

Nanostructured materials are most important materials studied during last decade. Usually these materials prepared from carbon. Because of the role of these materials in new technology, it is important to investigate their mathematical properties [1].

Let *G* be a graph with vertex set $V(G)$ and edge set $E(G)$. An automorphism of *G* is a one-to-one correspondence α: $V(G) \longrightarrow V(G)$ such that for every vertex *x* and *y* of *G*, *x* is adjacent to *y* if and only if $\alpha(x)$ is adjacent to $\alpha(y)$. A topological index for *G* is a real number invariant under the automorphisms of *G*. Obviously, the numbers of atoms and the numbers of bonds in a molecular graph are topological index. Such numbers based on the degrees of vertices are widely used for establishing relationships between the structure of molecules and their physico-chemical properties.

We now recall some algebraic notations that will be used in the paper. If *e* is an edge of *G*, connecting the vertices *u* and *v* then we write $e = uv$. The distance between a pair of vertices *u* and *w* of *G* is denoted by $d(u,w)$. The first non trivial distance-based topological index was introduced early by Wiener [2]. He defined his index as the sum of distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds. We encourage the reader to consult papers [3,4] and references therein, for further study on the topic.

Following Vukičević and Furtula [5] the *GA* index of a molecular graph *G* is defined as $GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{deg(u)deg(v)}}{deg(u)+deg(v)}$, where $deg(u)$ denotes the degree of vertex *u* in *G* and sum is taken over all unordered pairs $\{u,v\}$ of distinct vertices in *G*. Another variant of this new proposed topological index was introduced by Fath-Tabar et al. [6].

The problem of computing topological indices of nanostructures was introduced firstly by Diudea and his co-authors [7-12] and then continued by one the present authors (ARA) [13-25]. We also encourage the readers to consult papers by Ghorbani et al. [26, 27] and Taeri and his co-workers [28, 29] for background material, as well as basic computational techniques.

In the present article, we take the polyhex armchair, polyhex zig-zag and TUC_4C_8(R/S) nanotubes into account and compute their *GA* index. Our notation is standard and mainly taken from the famous books of Trinajestic [30] and West [31] and other standard books on graph theory. The graphs P_n and C_n denote the path and cycle with *n* vertices.

2. Main results

In this section we derive exact formulas for the *GA* index of nanotubes and nanotori constructed by hexagons, squares-octagons and rhombs-octagons, Figs. 1-4. To explain these nanotubes, we must present some algebraic notations. If G and H are graphs such that $V(G) \subseteq V(H)$ and $E(G) \subseteq E(H)$ then we say G is a subgraph of H. For given graphs G_1 and G_2 their Cartesian product $G_1 \square G_2$ is defined as the graph on the vertex set $V(G_1) \times V(G_2)$ with vertices $u = (u_1,u_2)$ and $v = (v_1,v_2)$ connected by an edge if and only if either $([u_1 = v_1 \text{ and } u_2v_2 \in E(G_2)])$ or $([u_2 = v_2 \text{ and } u_1v_1 \in E(G_1)])$.

Suppose $A[m,n]$ denotes an armchair polyhex nanotube with m + 1 rows and n columns; see Figs. 1 and 5. Then $A[m,n]$ is a subgraph of $C_n \times P_m$, where *n* is even. It is easily seen that $|V(A[m,n])| = mn$ and $|E(A[m,n])| = 3/2\times mn$. In a similar way, the zig-zag polyhex nanotube $Z[m,n]$, Figs. 2 and 6, is also a subgraph of $C_n \times P_m$, where *n* is even. In this case $|V(Z[m,n])| = mn$ and $|E(Z[m,n])| = 3/2\times mn - n/2$. The TUC_4C_8(R) nanotube $R[m,n]$ is our third class of nanotubes constructed from rhombs and octagons, Fig. 3, where *m* and *n* are the number of quadrangles in each rows and columns, respectively. It is obtained from $C_m \times P_n$ by replacing each vertex by rhombus. Obviously $|V(R[m,n])| = 4mn$ and $|E(R[m,n])| = 6mn$.

Fig. 1. An Armchair Polyhex Nanotube A[m,n].

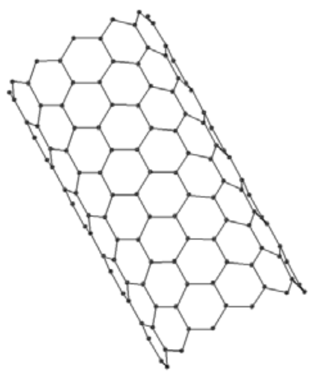

Fig. 2. An Armchair Polyhex Nanotube Z[m,n].

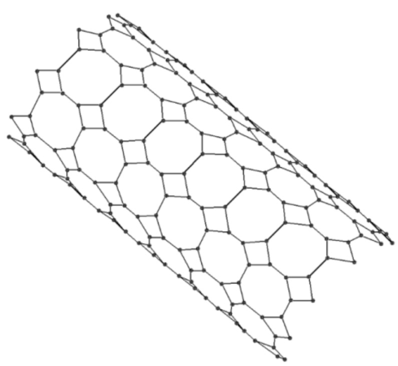

Fig. 3. $TUC_4C_8(R)[m,n]$ Nanotube.

Fig. 4. $TUC_4C_8(S)[m,n]$ Nanotube.

The forth class of nanotubes is $TUC_4C_8(S)[m,n]$. This class of nanotubes is constructed from squares and rhombs. It is easy to see that this nanotubes is a subgraph of $C_n \times P_m$, where n is even. Clearly, $|V(S[m,n])| = mn$ and $|E(S[m,n])| = 3/2\times mn - n/2$, Figs. 4 and 7.

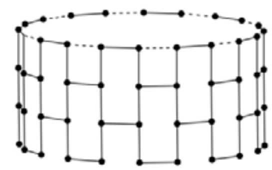

Fig. 5. The Armchair Nanotube A[3,20].

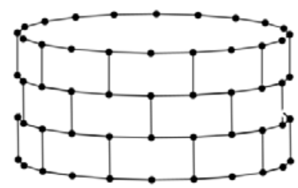

Fig. 6. The Armchair Nanotube Z[3,20].

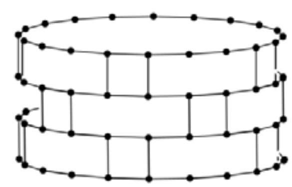

Fig. 7. The $TUC_4C_8(S)$ Nanotube S[3,20].

If G is a nanotorus of above types then one can easily seen that G is 3-regular and so their Geometric-Arithmetic index is equal to the number of their edges, i.e. $GA(G) = |E(G)|$. On the other hand, by counting vertices of degree 2, we have:

$$GA(A[m,n]) = n\left[\frac{3m}{2} + \frac{4\sqrt{6}}{5} - 2\right],$$

$$GA(Z[m,n]) = n\left[\frac{3m}{2} + \frac{4\sqrt{6}}{5} - \frac{5}{2}\right],$$

$$GA(R[m,n]) = 2n\left[3m + \frac{4\sqrt{6}}{5} - 2\right],$$

$$GA(S[m,n]) = n\left[\frac{3m}{2} + \frac{2\sqrt{6}}{5} - \frac{3}{2}\right].$$

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• Corresponding author: Ashrafi@kashanu.ac.ir