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GEOMETRIC–ARITHMETIC INDEX: AN ALGEBRAIC APPROACH

HOSSEIN SHABANI[a], ALI REZA ASHRAFI[a*], IVAN GUTMAN[b]

ABSTRACT. The *Geometric-Arithmetic* (*GA*) index is a recently proposed topological index in mathematical chemistry. In this paper, a group theoretical method for computing the *GA* index of graphs is presented. We apply this method to some classes of dendrimers to calculate their *GA* index.

Keywords: *geometric-arithmetic index, dendrimer*

INTRODUCTION

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted. By IUPAC terminology, a topological index is a numerical value associated with a chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity [1–3]. The name "topological index" was first used by Hosoya [4], in connection with his *Z* index, which he used for characterizing the topological nature of graphs.

A dendrimer is generally described as a macromolecule, which is built up from a starting atom, such as nitrogen, to which carbon and other elements are added by a repeating series of chemical reactions that produce a spherical branching structure. In a divergent synthesis of a dendrimer, one starts from the core (a multi connected atom or group of atoms) and growths out to the periphery. In each repeated step, a number of monomers are added to the actual structure, in a radial manner, resulting in quasi concentric shells, called generations. In a convergent synthesis, the periphery is first built up and next the branches (called dendrons) are connected to the core. The stepwise growth of a dendrimer follows a mathematical progression and its size is in the nanometer scale [5–7].

We now recall some algebraic notations that will be used throughout. Suppose G is a graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. If e is an edge of G, connecting the vertices u and v then we write $e = uv$. For each vertex a and b, $d(a,b)$ denotes the length of a minimal path connecting them. The eccentricity of a vertex x, $\varepsilon(x)$, is defined as the maximum of $\{d(y,x) \mid y \in V(G)\}$.

[a] *Department of Mathematics, Statistics and Computer Science, Faculty of Science, University of Kashan, Kashan 87317-51167, I. R. Iran*
[b] *Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia*

Following Vukičević and Furtula [8], 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 the sum is taken over all edges *e* = *uv* of *G*. We encourage the interested readers to consult the papers [9–16] for other variants of this new topological index and their mathematical properties, as well as the reviews [17,18].

In the present article, we continue our works on computing the topological indices of dendrimers [19–21]. Our notation is standard and mainly taken from the standard books of graph theory.

RESULTS AND DISCUSSION

The *GA* index of a molecular graph *G* is based on ratio of the geometric and arithmetic mean and can be computed by considering the automorphism group of *G*. One method to calculate this topological index efficiently is to use group theory and in particular the automorphism group of the graph [23–26]. An automorphism of a graph *G* is an isomorphism of *G* with itself and the set of all such mappings is denoted by *Aut*(*G*).

Figure 1. The All-Aromatic Dendrimer $DNS_1[1]$ and $DNS_1[3]$, respectively.

Figure 2. The Wang's Helicene-Based Dendrimers $DNS_2[2]$ and $DNS_2[3]$, respectively.

In mathematics, groups are often used to describe symmetries of objects. This is formalized by the notion of a group action: every element of the group "acts" like a bijective map (or "symmetry") on some set. To clarify this notion, we assume that *Γ* is a group and *X* is a set. *Γ* is said to act on *X* when there is a map $\phi : \Gamma \times X \longrightarrow X$ such that all elements $x \in X$, (i) $\phi(e,x) = x$ where e is the identity element of Γ, and (ii) $\phi(g, \phi(h,x)) = \phi(gh,x)$ for all $g,h \in \Gamma$. In this case, Γ is called a transformation group; X is called a Γ-set, and ϕ is called the group action. For simplicity we define $gx = \phi(g,x)$.

In a group action, a group permutes the elements of X. The identity does nothing, while a composition of actions corresponds to the action of the composition. For a given X, the set $\{gx \mid g \in \Gamma\}$, where the group action moves x, is called the group orbit of x. The subgroup which fixes is the isotropy group of x.

Let H and K be two groups and K acts on a set X. The wreath product H~K of these groups is defined as the set of all order pair (f ; k), where $k \in K$ and $f : X \to H$ is a function such that $(f_1 ; k_1).(f_2 ; k_2) = (g ; k_1k_2)$ and $g(i) = f_1(i) f_2(i^{k_2})$.

In the following simple lemma a formula for computing the *GA* index of a graph based on the action of *Aut*(*G*) on *E*(*G*) is obtained.

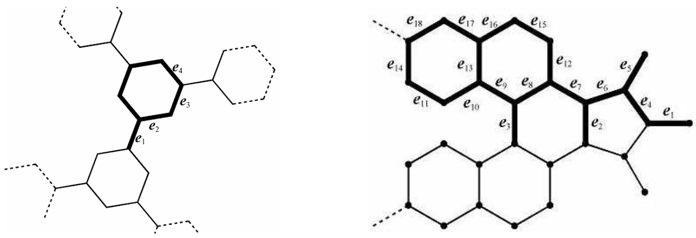

Figure 3. Some Elements of $E_{i,1}$, $E_{i,2}$, $E_{i,3}$, $E_{i,4}$ and .

Lemma. Consider the natural action of *Aut*(*G*) on the set of edges containing orbits E_1, E_2, … , E_k. Then $GA(G) = \sum_{i=1}^{k} |E_i| \frac{2\sqrt{deg(u_i)deg(v_i)}}{deg(u_i) + deg(v_i)}$, where u_iv_i is an edge of the i–th orbit. In particular, if the action is transitive and $e=uv$ is an edge of G then $GA(G) = |E(G)| \frac{2\sqrt{deg(u)deg(v)}}{deg(u) + deg(v)}$.

Proof. By definition, for each edge $e_1=uv$ and $e_2=xy$ in the same orbit O, there exists an automorphism f such that ($f(u)=x$ & $f(v)=y$) or ($f(u)=y$ & $f(v)=x$). Thus $\frac{2\sqrt{deg(u)deg(v)}}{deg(u) + deg(v)} = \frac{2\sqrt{deg(x)deg(y)}}{deg(x) + deg(y)}$. Since $E(G)$ is partitioned by orbits, $GA(G) = \sum_{i=1}^{k} \sum_{uv \in E_i} \frac{2\sqrt{deg(u)deg(v)}}{deg(u) + deg(v)} = \sum_{i=1}^{k} |E_i| \frac{2\sqrt{deg(u_i)deg(v_i)}}{deg(u_i) + deg(v_i)}$. This completes the proof.

We are now ready to calculate the *GA* index of dendrimers depicted in Figures 1 to 3. We have:

Theorem. The *GA* indices of dendrimers depicted in Figures 1 and 2 are as follows:

1. $GA(DNS_1[n]) = 9\times 2^n + 24(2^n - 1)\sqrt{6}/5 - 3,$
2. $GA(DNS_2[n]) = 2^{n-1}(22 + 16\sqrt{6}/5 + 2\sqrt{3}) - (2^{n-1} - 1)(19 + 24\sqrt{6}/5 + 2\sqrt{3}) + (\sqrt{3} - 1).$

Proof. To compute the *GA* indices of these dendrimers, we first compute the number of their vertices and edges as follows:

$|V(DNS_1[n])| = 18 \times 2^{n+1} - 12$; $|V(DNS_2[n])| = 27\times 2^{n+1} - 1$
$|E(DNS_1[n])| = 21 \times 2^{n+1} - 15$; $|E(DNS_2[n])| = 33(2^{n+1} - 1)$

Next we compute the automorphism group of $DNS_1[n]$. To do this, we assume that $T[n]$ is a graph obtained from $DNS_1[n]$ by contracting each hexagon to a vertex. The adjacencies of these vertices are same as the adjacencies of hexagons in $DNS_1[n]$. Choose the vertex x_0 of $T[n]$, associated to the central hexagon, as root. Label vertices of $T[n]$ adjacent to x_0 by 1, 2 and 3; the vertices with distance 2 from x_0 by 4, 5, 6, 7, 8, 9; the vertices with distance 3 from x_0 by 10, 11, 12, …, 21; … and vertices with distance n from x_0 by $3 \times (2^n-1) + 1, \ldots, 3 \times (2^{n+1}-1)$. Set $X = \{1, 2,\ldots, 3\times(2^{n+1}-1)\}$. Then S_3 acts on $X = \{1, 2, \ldots, 3\times(2^n-1)\}$ and the automorphism group of $DNS_1[n]$ is isomorphic to $Z_2 \sim S_3$, obtained from above action, see Figure 3. Suppose $Aut(DNS_1[n])$ acts on $E(DNS_1[n])$ and $E_{0,0}$, $E_{1,1}$, $E_{1,2}$, $E_{1,3}$, $E_{1,4}$, …, $E_{n,1}$, $E_{n,2}$, $E_{n,3}$, $E_{n,4}$ are orbits of this action. We also assume that H is the central hexagon and $E_{0,0}$ is the set of all edges of H. To obtain the edges $E_{i,1}$, $E_{i,2}$, $E_{i,3}$, $E_{i,4}$ we use the following algorithm:

1. $E_{i,1}$ is the set of all edges $e = uv$ such that $d(u,H) = 3i - 3$, $d(v,H) = 3i - 2$ and $\deg(u) = \deg(v) = 3$, where for each subset $Y \subseteq V(DNS_1[n])$, $d(u,Y) = Min\{d(u,b) \mid b \in Y\}$.
2. $E_{i,2}$ is the set of all edges $e = uv$ such that $d(u,H) = 3i - 2$ and $d(v,H) = 3i - 1$.
3. $E_{i,3}$ is the set of all edges $e = uv$ such that $d(u,H) = 3i - 1$ and $d(v,H) = 3i$.
4. $E_{i,4}$ is the set of all edges $e = uv$ such that $d(u,H) = 3i$, $d(v,H) = 3i + 1$, $deg(u) = 3$ and $deg(v) = 2$.

Obviously, for $DNS_1[n]$ if $e = uv \in E_{i,j}$ then

$$\frac{2\sqrt{deg(u)deg(v)}}{deg(u)+deg(v)} = \begin{cases} 1 & i=1 \\ 2\sqrt{6}/5 & i=2,3,4 \end{cases}.$$

Moreover, $|E_{i,1}| = 3 \times 2^{i-1}$ and $|E_{i,2}| = |E_{i,3}| = |E_{i,4}| = 6 \times 2^{i-1}$. This completes the proof of (1). To prove 2, it is enough to consider the action of the group $Aut(DNS_2[n])$

on $E(DNS_2[n])$ and use a similar method as given the case 1. Notice that in this case the automorphism group $Aut(DNS_2[n])$ is isomorphic to the wreath product $Z_2 \sim Z_2$, where Z_2 acts on the set $Z = \{1, 2, \ldots, 2^n-1\}$.

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