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GA index of nanostar dendrimers

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Let Σ be the class of finite graphs. A topological index is a function Top from Σ into real numbers with this property that Top(G) = Top(H), if G and H are isomorphic. Let G be a graph and e = uv be an edge of G. The GA index of G is defined as $GA(G) = \sum_{e\in E} \frac{2\sqrt{dudv}}{du+dv}$. In this paper we compute some results about this new topological index.

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1. Introduction

Dendrimers are macromolecular nanoscale objects that are widely recognized as precise, mathematically defined, covalent core-shell assemblies. Since dendrimers are well defined organic molecules in the size range of (1 to 15) nm and are known to act as hosts for guest molecules, they are promising candidates as templates for the formation of inorganic nanoclusters [1,2].

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics [3-5]. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [6]. This theory had an important effect on the development of the chemical sciences.

Let G = (V , E) be a graph with finite vertex set V and edge set E. An edge (v,w) $\in$ E(G) is directed if $wv \notin E$ and undirected if wv $\in$ E. We denote a directed edge vw by v → w and write v − w if v w is undirected. If vw $\in$ E then v and w are adjacent. If v → w then v is a parent of w, and if v − w then v is a neighbor of w.

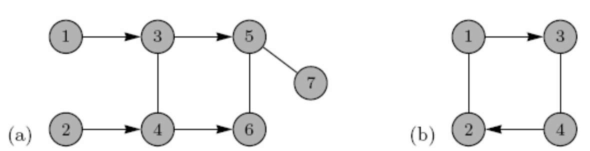

Fig. 1. (a) Chain graph with chain components {1}, {2}, {3, 4} and {5, 6, 7}; (b) a graph that is not a chain graph.

A path in G is a sequence of distinct vertices $<v_0, \ldots, v_k>$ such that v_{i-1} and v_i are adjacent for all $1 \le i \le k$. A path $<v_0, \ldots, v_k>$ is a semi-directed cycle if $v_iv_{i+1} \in E$ for all $0 \le i \le k$ and at least one of the edges is directed as $v_i \to v_{i+1}$. Here, $v_{k+1} \equiv v_0$. A chain graph is a graph without semi-directed cycles.

The GA index of G was introduced by D. Vukičevič and co-authors[7] as $GA(G) = \sum_{e=uv\in E(G)} \frac{2\sqrt{dudv}}{du+dv}$ in which, du denoted to the degree of vertex u. In this paper we compute GA index for chain graphs. Herein, our notation is standard and taken from the standard book of graph theory [8-22].

2. Main results and discussion

The aim of this section is to compute the GA index of nanostar dendrimers. Before going to calculate this index for nanostar dendrimers, we must compute GA index, for some well-known class of graphs.

Example 1. Consider the ladder graph L_n, with $2n$ vertices (figure 2). It is easy to see that $GA(L_n) = 4n - 8 + \frac{8\sqrt{6}}{5}$.

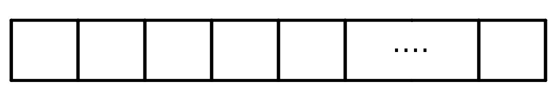

Fig. 2. Graph of ladder with 2n vertices.

Example 2. Let W_n denoted the wheel graph on $n+1$ vertices (figure 3). We know that the central vertex is of degree n and other vertices are of degree 3. So, we have: $GA(W_n) = n + \frac{2n\sqrt{3n}}{3+n}$.

Example 3. Let $GP(n,k)$ be generalized Petersen graph with parameters n and k, vertex set $V=\{x_1,...,x_n,y_1,...,y_n\}$ and edge set $E=\{x_1x_2,x_2x_3,...,x_nx_1,x_1y_1,x_2y_2,...,x_ny_n,y_1y_{k+1},y_2y_{k+2},...,y_ny_{k+n}\}$ (mod n) respectively. It is easy to see that $|E(GP(n,k))|=\begin{cases}3n & \text{if } n\neq 2k\\ \frac{5n}{2} & \text{if } n=2k\end{cases}$ and so, we have

$$GA(GP(n,k))=\begin{cases}3n & \text{if } n\neq 2k\\ \frac{3n}{2}+\frac{2n\sqrt{6}}{5} & \text{if } n=2k\end{cases}.$$

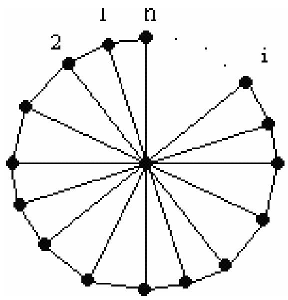

Fig. 3. Graph of wheel on n + 1 vertices.

Example 3. Let C_n be a cycle on n vertices. We know all of vertices are of degree 2. So, we have

$$GA(G)=\sum_{e\in E}\frac{2\sqrt{2\times 2}}{2+2}=n.$$

Now let $GA^{(a_1,...,a_n)}(G)=\sum_{\substack{uv\in E(G)\\ u,v\neq a_1,...,a_n}}\frac{2\sqrt{du\,dv}}{du+dv}$, $a_i\in V(G)$ $(1\leq i\leq n)$. By this notation we have:

Lemma 1: Suppose $G=G(G_1,G_2,...,G_n,v_1,v_2,...,v_n)$ be a chain graph. So, we have:

(i)

$$|V(G(G_1,G_2,...,G_n,v_1,v_2,...,v_n))|=\sum_{i=1}^{n}|V(G_i)|,$$

(ii)

$$|E(G(G_1,G_2,...,G_n,v_1,v_2,...,v_n))|=\sum_{i=1}^{n}|E(G_i)|+n-1,$$

(iii) $G(G_1,G_2,...,G_n,v_1,v_2,...,v_n)$ is connected if and only if G_i $(1\leq i\leq n)$ be connected,

(iv) $d_G\,a=\begin{cases}d_{G_i}\,a & a\in V(G_i) \text{ and } a\neq v_i\\ d_{G_i}\,a+1 & a=v_i,\ i=1,n\\ d_{G_i}\,a+2 & a=v_i,\ 2\leq i\leq n-1\end{cases}.$

Proof. The proof is straightforward.

Theorem 2. For the chain graph $G=G(G_1,G_2,v_1,v_2)$ we have:

$$GA(G)=\sum_{i=1}^{2}(GA^{(v_i)}(G)+\sum_{j=1}^{d_{G_i}v_i}\frac{2\sqrt{(d_{G_i}\,v_i+1)\,d_{G_i}\,u_{ij}}}{d_{G_i}\,v_i+d_{G_i}\,u_{ij}+1}) + \frac{2\sqrt{(d_{G_1}\,v_1+1).(d_{G_2}\,v_2+1)}}{d_{G_1}\,v_1+d_{G_2}\,v_2+2}$$

in which vertices u_{ij} and v_i are adjacent.

Proof.

$$GA(G)=\sum_{\substack{uv\in E(G)\\ u,v\neq v_1,v_2}}\frac{2\sqrt{du\,dv}}{du+dv}+\sum_{\substack{uv_1\in E(G)\\ u\neq v_2}}\frac{2\sqrt{du\,dv_1}}{du+dv_1}+\sum_{\substack{uv_2\in E(G)\\ u\neq v_1}}\frac{2\sqrt{du\,dv_2}}{du+dv_2}+\frac{2\sqrt{dv_1\,dv_2}}{dv_1+dv_2}=$$

$$\sum_{i=1}^{2}(GA^{(v_i)}(G)+\sum_{j=1}^{d_{G_i}v_i}\frac{2\sqrt{(d_{G_i}\,v_i+1)\,d_{G_i}\,u_{ij}}}{d_{G_i}\,v_i+d_{G_i}\,u_{ij}}+\frac{2\sqrt{(d_{G_1}\,v_1+1).(d_{G_2}\,v_2+1)}}{d_{G_1}\,v_1+d_{G_2}\,v_2+2}).$$

Theorem 3. Consider the chain graph $G=G(G_1,G_2,...,G_n,v_1,v_2,...,v_n)$ $(n\geq 3)$. We have:

$$GA(G)=\sum_{i=1}^{n}GA^{(v_i)}(G_i)+\sum_{i=2}^{n-1}\sum_{j=1}^{d_{G_i}v_i}\frac{2\sqrt{(d_{G_i}\,v_i+2)\,d_{G_i}\,u_{ij}}}{d_{G_i}\,v_i+d_{G_i}\,u_{ij}+2}+\sum_{i=1,n}\sum_{j=1}^{d_{G_i}v_i}\frac{2\sqrt{(d_{G_i}\,v_i+1)\,d_{G_i}\,u_{ij}}}{d_{G_i}\,v_i+d_{G_i}\,u_{ij}+1}$$

$$+\sum_{i=2}^{n-1}\frac{2\sqrt{(d_{G_i}\,v_i+2)(d_{G_{i+1}}\,v_{i+1}+2)}}{d_{G_{i+1}}\,v_i+d_{G_{i+1}}\,v_{i+1}+4}+\frac{2\sqrt{(d_{G_1}\,v_1+1).(d_{G_2}\,v_2+2)}}{d_{G_1}\,v_1+d_{G_2}\,v_2+3}+\frac{2\sqrt{(d_{G_{n-1}}\,v_{n-1}+2).(d_{G_n}\,v_n+1)}}{d_{G_{n-1}}\,v_{n-1}+d_{G_n}\,v_n+3},$$

in which vertices u_{ij} are adjacent to the vertices v_i.

Proof. $$GA(G)=\sum_{\substack{uv\in E(G)\\ u,v\neq v_1,\ldots,v_n}}\frac{2\sqrt{du\,dv}}{du+dv}+\sum_{i=1}^{n}\sum_{\substack{uv_i\in E(G)\\ u\neq v_1,\ldots,v_n}}\frac{2\sqrt{du\,dv_i}}{du+dv_i}+\sum_{i=1}^{n-1}\sum_{v_iv_{i+1}\in E(G)}\frac{2\sqrt{dv_i\,dv_{i+1}}}{dv_i+dv_{i+1}}=$$

$$\sum_{i=1}^{n}GA^{(v_i)}(G_i)+\sum_{i=2}^{n-1}\sum_{j=1}^{d_{G_i}v_i}\frac{2\sqrt{(d_{G_i}v_i+2)d_{G_i}u_{ij}}}{d_{G_i}v_i+d_{G_i}u_{ij}+2}+$$

$$\sum_{i=1,n}\sum_{j=1}^{d_{G_i}v_i}\frac{2\sqrt{(d_{G_i}v_i+1)d_{G_i}u_{ij}}}{d_{G_i}v_i+d_{G_i}u_{ij}+1}+$$

$$\sum_{i=2}^{n-1}\frac{2\sqrt{(d_{G_i}v_i+2)(d_{G_{i+1}}v_{i+1}+2)}}{d_{G_{i+1}}v_i+d_{G_{i+1}}v_{i+1}+4}+$$

$$\frac{2\sqrt{(d_{G_1}v_1+1)(d_{G_2}v_2+2)}}{d_{G_1}v_1+d_{G_2}v_2+3}+$$

$$\frac{2\sqrt{(d_{G_{n-1}}v_{n-1}+2)(d_{G_n}v_n+1)}}{d_{G_{n-1}}v_{n-1}+d_{G_n}v_n+3}.$$

Example 4. Consider the graph G_1 shown in figure 4. It is easy to see that $GA(G_1)=15+\frac{12\sqrt{6}}{5}$, $GA^{(v_i)}(G_1)=13+\frac{12\sqrt{6}}{5}$ and $GA^{(v_i,v_j)}(G_1)=11+\frac{12\sqrt{6}}{5}$ $(1\le i\ ,\ j\le 3,\ i\neq j)$.

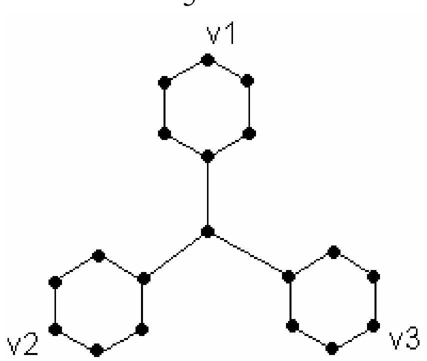

Fig. 4. Graph of nanostar dendrimer for n = 1.

Example 5. Consider the nanostar dendrimer shown in figure 5. One can see that:

$$G_n=G(G_{n-1},G_1,v,v),$$

$$GA(G_n)=GA^{(v)}(G_{n-1})+GA^{(v)}(G_1)+c,$$

$$GA^{(v)}(G_{n-1})=GA^{(v)}(G_{n-2})+GA^{(v,v)}(G_1)+c,$$

$$GA^{(v)}(G_{n-2})=GA^{(v)}(G_{n-3})+GA^{(v,v)}(G_1)+c,$$

$$\vdots$$

$GA^{(v)}(G_2)=GA^{(v)}(G_1)+GA^{(v,v)}(G_1)+c$ in which $c=1+\frac{8\sqrt{6}}{5}$ and so we have $GA(G_n)=2GA^{(v)}(G_1)+(n-2)GA^{(v,v)}(G_1)+(n-1)(1+\frac{8\sqrt{6}}{5})$. Now by summation of these relations one can see that $GA(G_n)=(20n-8)\frac{\sqrt{6}}{5}+12n+3$.

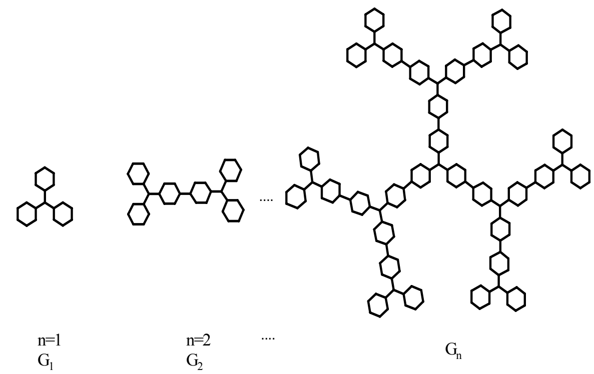

Fig. 5. Graph of nanostar dendrimer.

References

[1] D. A. Tomalia, A. M. Naylor, W. A. Goddard, Angew. Chem., **102,** 119 (1990).
[2] D. A. Tomalia, D. M. Hedstrand, M. S. Ferritto, Macromol. **24** (1991) 1435.
[3] N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton, FL 1992.
[4] I. Gutman, O. E. Polansky. Mathematical Concepts in Organic Chemistry, Springer-Verlag, New York, 1986.
[5] M. A. Johnson, G. M. Maggiora, Concepts and Applications of Molecular Similarity, Wiley Interscience, New York 1990.
[6] P. E. John, A. E. Vizitiu, S. Cigher, M. V. Diudea, MATCH Commun. Math. Comput.Chem. **57**, 479 (2007).
[7] D. Vukičevič, B. Furtula, J. Math. Chem., (2009), (DOI 10.1007/s10910-009-9520-x).
[8] M. Ghorbani, M. Jalal-Abadi, Iranian Journal of Mathematics and Sciences and Informatics **2**(2), 61 (2007).
[9] A. R. Ashrafi, M. Ghorbani, Digest Journal of Nanomaterials and Biostructures, **4**(2), 313 (2009).
[10] A. R. Ashrafi, M. Ghorbani, M. Jalali, J. Theo. Com. Chem., **8**(3), 451 (2009)

[11] A. R. Ashrafi, M. Ghorbani, M. Hemmasi, Digest Journal of Nanomaterials and Biostructures **4**(3), 483 (2009).
[12] A. R. Ashrafi, M. Ghorbani, Digest Journal of Nanomaterials and Biostructures, **4**(2), 389 (2009).
[13] M. Ghorbani, M. B. Ahmadi, M. Hemmasi, Digest Journal of Nanomaterials and Biostructures **3**(4), 269 (2009)
[14] M. Ghorbani, M. Jalali, Digest Journal of Nanomaterials and Biostructures, **4**(1), 177 (2009).
[15] M. Ghorbani, M. Jalali, Digest Journal of Nanomaterials and Biostructures**,** **4**(3), 403 (2009).
[16] M. Ghorbani, M. Jalali, MATCH Commun. Math. Comput. Chem., **62**, 353 (2009).
[17] A. R. Ashrafi, M. Ghorbani, International Journal of Computer Mathematics, (2009) Accepted.
[18] A. R. Ashrafi, M. Ghorbani, Fullerenes, Nanotubes and Carbon Nanostructures, (2009) Accepted.
[19] M. Ghorbani, M. Jalali, Studia universitatis babes – Bolay, chemia, **2**, 145 (2009).
[20] M. Ghorbani, M. Jalali, Digest Journal of Nanomaterials and Biostructures **4**(2), 423 (2009).
[21] A. R. Ashrafi, M. Ghorbani, M. Jalali, Optoelectron. Adv. Mater. - Rapid Comm. **3**(8), 823 (2009).
[22] A. R. Ashrafi and M. Ghorbani, Optoelectron. Adv. Mater. - Rapid Comm. **3**(6), 596 (2009).

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