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Computing fifth geometric-arithmetic index for nanostar dendrimers

ANTE GRAOVAC, MODJTABA GHORBANI• AND MOHAMMAD A. HOSSEINZADEH

Institute R. Bošković, HR-10002 Zagreb, POB 180, Croatia, and Faculty of Science, University of Split Nikole Tesle 12, HR-21000, Split, Croatia
Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785 – 136, I. R. Iran;
Corresponding author: mghorbani@srttu.edu

ABSTRACT. The geometric-arithmetic index is a topological index was defined as $GA(G)=\sum_{uv\in E}\frac{2\sqrt{d_u d_v}}{d_u+d_v}$, in which degree of vertex u denoted by $d_G(u)$. Now we define a new version of *GA* index as $GA_5(G)=\sum_{e=uv\in E(G)}\frac{2\sqrt{\delta_u\delta_v}}{\delta_u+\delta_v}$, where $\delta_u=\sum_{uv\in E(G)} d_v$. The goal of this paper is to further the study of the GA_5 index.

Keywords: GA index, GA_5 index, Dendrimers.

1. INTRODUCTION

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. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena. This theory has an important effect on the development of the chemical sciences.

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 chemical

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•Author to whom correspondence should be addressed.(e-mail:mghorbani@srttu.edu) constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity.

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. If e is an edge of G, connecting the vertices u and v, then we write $e = uv$ and say "u and v are adjacent". A connected graph is a graph such that there is a path between all pairs of vertices.

Let $\sum$ be the class of finite graphs. A topological index is a function Top from $\sum$ into real numbers with this property that $Top(G) = Top(H)$, if G and H are isomorphic. Obviously, the number of vertices and the number of edges are topological index. The Wiener [1] index is the first reported distance based topological index and is defined as half sum of the distances between all the pairs of vertices in a molecular graph. If $x, y \in V(G)$ then the distance $d_G(x,y)$ between x and y is defined as the length of any shortest path in G connecting x and y.

A class of geometric–arithmetic topological indices [2] may be defined as $GA_{general} = \sum_{uv\in E}\frac{2\sqrt{Q_uQ_v}}{Q_u+Q_v}$, where Q_u is some quantity that in a unique manner can be associated with the vertex u of the graph G. The first member of this class was considered by Vukicevic and Furtula [3], by setting Q_u to be the

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

in which degree of vertex u denoted by $d_G(u)$. The second member of this class was considered by Fath-Tabar et al. [4] by setting Q_u to be the number n_u of vertices of G lying closer to the vertex u than to the vertex v for the edge uv of the graph G:

$$GA_2(G) = \sum_{uv\in E}\frac{2\sqrt{n_un_v}}{n_u+n_v}.$$

The third member of this class was considered by Bo Zhou et al.[5] by setting Q_u to be the number m_u of edges of G lying closer to the vertex u than to the vertex v for the edge uv of the graph G:

$$GA_3(G) = \sum_{uv\in E}\frac{2\sqrt{m_um_v}}{m_u+m_v}.$$

The fourth member of this class was considered by Ghorbani et al.[6] by setting Q_u to be the number ε_u the eccentricity of vertex u:

$$GA_4(G) = \sum_{uv\in E}\frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}.$$

Here, we define the fourth member of this class as follows:

$$GA_5(G) = \sum_{uv\in E} \frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)},$$

in which $\delta_G(u) = \sum_{uv\in E(G)} d_G(v)$.

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstić [7]. They are defined as:

$$M_1(G) = \sum_{v\in V(G)} (\deg_G(v))^2 \text{ and } M_1(G) = \sum_{uv\in E(G)} \deg_G(u)\deg_G(v).$$

Now we define a new version of Zagreb indices as follows:

$$M_1^{'}(G) = \sum_{uv\in E(G)} \delta_G(u)+\delta_G(v) \text{ and } M_2^{'}(G) = \sum_{uv\in E(G)} \delta_G(u)\delta_G(v).$$

Here our notations are standard and mainly taken from [8 – 13].

2. MAIN RESULTS AND DISCUSSION

The goal of this section is the study of GA5 index. Furthermore we compute some bounds for this new topological index.

Example 1. Let K_n be the complete graph on n vertices. Then for every $v\in V(K_n)$ and $\deg_G(v) = n-1$ and so $\delta_G(v) = (n-1)^2$. This implies that $GA_5(K_n) = n(n-1)/2$.

Example 2. Let C_n denote the cycle of length *n*. Then $d_G(v) = 2$ and $\delta_G(v) = 4$. Hence, $GA_5(C_n) = n$.

Example 3. Let P_n be a path of length *n*. Then one can see that

$$GA_5(P_n) = \frac{4\sqrt{6}}{5} + \frac{4\sqrt{3}}{7}(n-3).$$

Example 4. Let S_n be a star graph with *n* + 1 vertices. Then $GA_5(S_n) = n(n-1)/2$.

Lemma 5. The first Zagreb index satisfies in the following equation:

$$M_1(G) = \sum_{v\in V(G)} \delta_G(v).$$

Proof. By using definition one can see that:

$$\sum_{v\in V(G)} \delta_G(u) = \sum_{u\in V(G)} \sum_{v\in N_G(u)} \deg_G(v) = \sum_{v\in V(G)} (\deg_G(v))^2 = M_1(G).$$

By using definition of GA5 index we can prove, $0 \le \frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)} \le 1$. So, we can conclude two following theorems:

Theorem 6. Let *G* be a non empty connected graph on *n* ≥ 3 vertices. Then

$$GA_5(G) \le \sqrt{M_2^{'} + 2M_2^{'2}}.$$

Proof. For every edge $e = uv$ in E(G), $\delta_G(u)+\delta_G(v)\geq 2$ and so we have:

$$(GA_5(G))^2 \leq \sum_{uv\in E(G)}\delta_G(u)\delta_G(v)+2\sum_{uv\neq u'v'}\sqrt{\delta_G(u)\delta_G(v)}\sqrt{\delta_G(u')\delta_G(v')}$$

$$\Rightarrow (GA_5(G))^2 \leq M_2^{'} + 2M_2^{'2} \Rightarrow GA_5(G) \leq \sqrt{M_2^{'}+2M_2^{'2}}.$$

Theorem 7. Let T be a chemical tree with n ≥ 2 vertices. Then $GA_5(T)\leq 256(n-1)$.

Proof. For every vertex $u\in V(T)$, deg(u) ≤ 4 and so, $\delta_G(u)\leq 4^4=256$. On the other hand, $\delta_G(u)+\delta_G(v)\geq 2$ and this completes the proof.

Theorem 8. Let Δ be the maximum degree of graph G. Then

$$\frac{1}{\Delta}GA(G)\leq GA_5(G)\leq \Delta GA(G).$$

Proof. For every vertex u in V(G) it is easy to see that $du\leq\delta_G(u)\leq\Delta du$.

An automorphism of the graph G = (V, E) is a bijection σ on V which preserves the edge set E, i. e., if $e = uv$ is an edge, then $\sigma(e)=\sigma(u)\sigma(v)$ is an edge of E. Here the image of vertex u is denoted by $\sigma(u)$. The set of all automorphisms of G under the composition of mappings forms a group which is denoted by Aut(G). Aut(G) acts transitively on V if for any vertices u and v in V there is $\alpha\in Aut(G)$ such that $\alpha(u)=v$. Similarly G = (V, E) is called edge-transitive graph if for any two edges $e_1 = uv$ and $e_2 = xy$ in E there is an element $\beta\in Aut(G)$ such that $\beta(e_1)=e_2$ where $\beta(e_1)=\beta(u)\beta(v)$. Let G = (V, E) be a graph. If Aut(G) acts edge-transitively on V, then we have the following Lemma:

Lemma 9. $GA_5(G)=|E|\dfrac{\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}$, for every $e=uv\in E(G)$.

Example 10. Let S_n be the star graph with n + 1 vertices. It is easy to see that S_n is edge-transitive. So we have:

$$GA_5(S_n)=n\times 1=n.$$

Lemma 11. Let G = (V, E) be a graph. If Aut(G) on E has orbits E_i, $1\leq i\leq s$, where $e_i=u_iv_i$ is an edge of G. then:

$$GA_5(G)=2\sum_{i=1}^{s}|E_i|\frac{\sqrt{\delta_G(u_i)\delta_G(v_i)}}{\delta_G(u_i)+\delta_G(v_i)}.$$

In this section we compute the truncated GA_5 index of the chain graphs. Then we use this method to compute the GA_5 index for an infinite class of nanostar dendrimers.

3. APPLICATIONS

In this section we compute GA_5 index of a class of nanostar dendrimer. To do this at first we introduce the concept of truncated GA_5 index. Let $U=\{u_1,u_2,\ldots,u_k\}$ be a subset of V(G). We now define a new version of the GA5 index and name it the truncated GA5 index $GA_5^{(U)}$ as

$$GA_5^{(u_1,u_2,\ldots,u_k)}(G)=\sum_{\substack{uv\in E(G)\\ u,v\notin\bigcup_{i=1}^{k}N_G[u_i]}}\frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}$$

i. e.,

$$GA_5^{(U)}(G)=\sum_{\substack{uv\in E(G)\\ u,v\notin\bigcup_{i=1}^{k}N_G[u_i]}}\frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}.$$

Where $N_G[u]=N_G(u)\cup\{u\}$.

It should be noticed that in the case $U = \emptyset$ then, $GA_5^{(U)}(G)=GA_5(G)$. Let G_i $(1 \le i \le n)$ be some graphs and $v_i \in V(G_i)$. A chain graph denoted by $G=G(G_1,\ldots,G_n,v_1,\ldots,v_n)$ is obtained from the union of the graphs G_i $(1 \le i \le n)$ by adding the edges v_iv_{i+1} $(1 \le i \le n-1)$, see Fig. 1. Then $|V(G)|=\sum_{i=1}^{n}|V(G_i)|$ and $|E(G)|=(n-1)+\sum_{i=1}^{n}|E(G_i)|$.

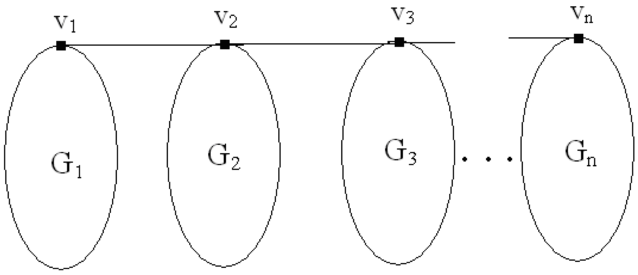

Fig. 1. The chain graph $G=G(G_1,\ldots,G_n,v_1,\ldots,v_n)$.

It is worth noting that the above specified class of chain graphs embraces, as special cases, all trees (among which are the molecular graphs of alkanes) and all unicyclic graphs (among which are the molecular graphs of monocycloalkanes). Also the molecular graphs of many polymers and dendrimers are chain graphs.

Lemma 12. Suppose that $G=G(G_1,G_2,\ldots,G_n,v_1,v_2,\ldots,v_n)$ is a chain graph. Then:

(i) $G=G(G_1,G_2,\ldots,G_n,v_1,v_2,\ldots,v_n)$ is connected if and only if G_i $(1\le i\le n)$ are connected.

$$\text{(ii) } \mathrm{d}_G(a)=\begin{cases}\mathrm{d}_{G_i}(a) & a\in V(G_i) \text{ and } a\neq v_i\\ \mathrm{d}_{G_i}(a)+1 & a=v_i,\ i=1,n\\ \mathrm{d}_{G_i}(a)+2 & a=v_i,\ 2\le i\le n-1\end{cases}.$$

(iii) if $u\in V(G_i)$ and $v_i\notin N_{G_i}[u]$ then $\delta_G(u)=\delta_{G_i}(u)$.

Theorem 13. If $n \geq 2$ and $v_1,...,v_n \neq u_1,...,u_k$, then for $G = G(G_1, G_2,...,G_n, v_1, v_2,...,v_n)$ it holds:

$$GA_5^{(u_1,...,u_k)}(G) = \sum_{i=1}^{n} GA_5^{(u_1,...,u_k,v_i)}(G_i) + \sum_{i=1}^{n} \sum_{\substack{uv\in E(G_i) \\ u\in N_{G_i}[v_i], \\ u,v\notin \bigcup_{i=1}^{k} N_G[u_i]}} \frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)} + \sum_{i=1}^{n-1} \frac{2\sqrt{\delta_G(v_{i-1})\delta_G(v_i)}}{\delta_G(v_{i-1})+\delta_G(v_i)}.$$

Proof. By using the definition of the truncated GA5 index one can see that

$$GA_5^{(u_1,u_2,...,u_k)}(G) = \sum_{\substack{uv\in E(G) \\ u,v\notin \bigcup_{i=1}^{k} N_G[u_i]}} \frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)} = \sum_{\substack{uv\in E(G) \\ u,v\notin \bigcup_{i=1}^{n} N_G[v_i] \cup \bigcup_{j=1}^{k} N_G[u_j]}} \frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}$$

$$+ \sum_{i=1}^{n} \sum_{\substack{uv\in E(G_i) \\ u\in N_{G_i}[v_i] \\ u,v\notin \bigcup_{i=1}^{k} N_G[u_i]}} \frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)} + \sum_{i=1}^{n-1} \frac{2\sqrt{\delta_G(v_{i-1})\delta_G(v_i)}}{\delta_G(v_{i-1})+\delta_G(v_i)}$$

$$= \sum_{\substack{uv\in E(G) \\ u,v\notin \bigcup_{i=1}^{n} N_G[v_i] \cup \bigcup_{j=1}^{k} N_G[u_j]}} \frac{2\sqrt{\delta_{G_i}(u)\delta_{G_i}(v)}}{\delta_{G_i}(u)+\delta_{G_i}(v)} + \sum_{i=1}^{n} \sum_{\substack{uv\in E(G_i) \\ u\in N_{G_i}[v_i] \\ u,v\notin \bigcup_{i=1}^{k} N_G[u_i]}} \frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}$$

$$+ \sum_{i=1}^{n-1} \frac{2\sqrt{\delta_G(v_{i-1})\delta_G(v_i)}}{\delta_G(v_{i-1})+\delta_G(v_i)} = \sum_{i=1}^{n} GA_5^{(u_1,...,u_k,v_i)}(G_i) + \sum_{i=1}^{n} \sum_{\substack{uv\in E(G_i) \\ u\in N_{G_i}[v_i] \\ u,v\notin \bigcup_{i=1}^{k} N_G[u_i]}} \frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)}$$

$$+ \sum_{i=1}^{n-1} \frac{2\sqrt{\delta_G(v_{i-1})\delta_G(v_i)}}{\delta_G(v_{i-1})+\delta_G(v_i)}.$$

Corollary 14. The truncated GA₅ index of the chain graph $G = G(G_1, G_2, v_1, v_2)$ $(v_1, v_2 \neq u_1,...,u_k)$ is:

$$GA_5^{(u_1,...,u_k)}(G) = \sum_{i=1}^{2} GA_5^{(u_1,...,u_k,v_i)}(G_i) + \sum_{i=1}^{2} \sum_{\substack{uv\in E(G_i) \\ u\in N_{G_i}[v_i] \\ u,v\notin \bigcup_{i=1}^{k} N_G[u_i]}} \frac{2\sqrt{\delta_G(u)\delta_G(v)}}{\delta_G(u)+\delta_G(v)} + \frac{2\sqrt{\delta_G(v_1)\delta_G(v_2)}}{\delta_G(v_1)+\delta_G(v_2)}.$$

We use from this corollary in the next section.

Example 15. Consider the graph G_1 shown in Fig. 2. It is easy to see that

$$GA_5(G_1) = \sqrt{35} + \frac{9\sqrt{7}}{8} + \frac{8\sqrt{5}}{3} + 6,$$

$$GA_5^{(v_1)}(G_1)=GA_5^{(v_2)}(G_1)=GA_5^{(v_3)}(G_1)=GA_5^{(v)}(G_1)=\sqrt{35}+\frac{9\sqrt{7}}{8}+\frac{16\sqrt{5}}{9}+4$$

and so,

$$GA_5^{(v,v)}(G_1)=GA_5^{(v_i,v_j)}(G_1)=\sqrt{35}+\frac{9\sqrt{7}}{8}+\frac{8\sqrt{5}}{9}+2,$$

for $1\le i,j\le 3, i\neq j$.

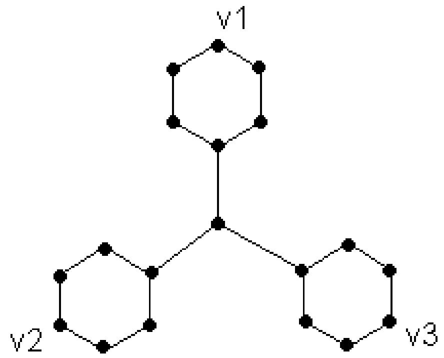

Fig. 2 The graph of nanostar G_n for n=1.

Consider now the chain graph $G_n=G(G_{n-1},H_1,v_1,u_1)$, shown in Fig. 2 (for $n=1$) and Fig. 3, respectively. It is easy to see that $H_i\cong G_1$ ($1\le i\le n$-1) and

$$G_n=G(G_{n-1},H_1,v_1,u_1)$$
$$G_{n-1}=G(G_{n-2},H_2,v_2,u_2)$$
$$\vdots$$
$$G_{n-i}=G(G_{n-i-1},H_{i+1},v_{i+1},u_{i+1})$$
$$\vdots$$
$$G_2=G(G_1,H_{n-1},v_{n-1},u_{n-1}).$$

Then by using corollary 3, we have the following relations:

$$GA_5(G_n)=GA_5^{(v_1)}(G_{n-1})+GA_5^{(u_1)}(H_1)+\frac{2\sqrt{35}}{3}+5$$
$$GA_5^{(v_1)}(G_{n-1})=GA_5^{(v_2)}(G_{n-2})+GA_5^{(v_1,u_2)}(H_2)+\frac{2\sqrt{35}}{3}+5$$
$$\vdots$$
$$GA_5^{(v_i)}(G_{n-i})=GA_5^{(v_{i+1})}(G_{n-i-1})+GA_5^{(v_i,u_{i+1})}(H_{i+1})+\frac{2\sqrt{35}}{3}+5$$
$$\vdots$$
$$GA_5^{(v_{n-2})}(G_2)=GA_5^{(v_{n-1})}(G_1)+GA_5^{(v_{n-2},u_{n-1})}(H_{n-1})+\frac{2\sqrt{35}}{3}+5.$$

Summation of these relations yields

$$GA_5(G_n) = GA_5^{(v_{n-1})}(G_1) + GA_5^{(u_1)}(H_1) + \sum_{i=2}^{n-1} GA_5^{(v_{i-1},u_i)}(H_i) + (n-1)(\frac{2\sqrt{35}}{3} + 5),$$

and so by using Example 1, it is easy to obtain

$$GA_5(G_n) = 2GA_5^{(v_1)}(G_1) + (n-2)GA_5^{(v_1,v_2)}(G_1) + (n-1)(\frac{2\sqrt{35}}{3} + 5)$$

$$= \left(\frac{5\sqrt{35}}{3} + \frac{9\sqrt{7}}{8} + \frac{8\sqrt{5}}{9} + 7\right)n - \frac{2\sqrt{35}}{3} + \frac{16\sqrt{5}}{9} - 1.$$

In other words we arrived at the following:

Theorem 16. Consider the chain graph $G_n = G(G_{n-1}, H_1, v_1, u_1)$ $(n \geq 2)$, shown in Fig. 3. Then,

$$GA_5(G_n) = \left(\frac{5\sqrt{35}}{3} + \frac{9\sqrt{7}}{8} + \frac{8\sqrt{5}}{9} + 7\right)n - \frac{2\sqrt{35}}{3} + \frac{16\sqrt{5}}{9} - 1.$$

Corollary 17. Consider the nanostar dendrimer D, shown in Fig. 4. Then,

$$GA_5(D) = \left(\frac{5\sqrt{35}}{3} + \frac{9\sqrt{7}}{8} + \frac{8\sqrt{5}}{9} + 7\right)n - \frac{2\sqrt{35}}{3} + \frac{16\sqrt{5}}{9} - 1.$$

where n is the number of repetition of the fragment G_1.

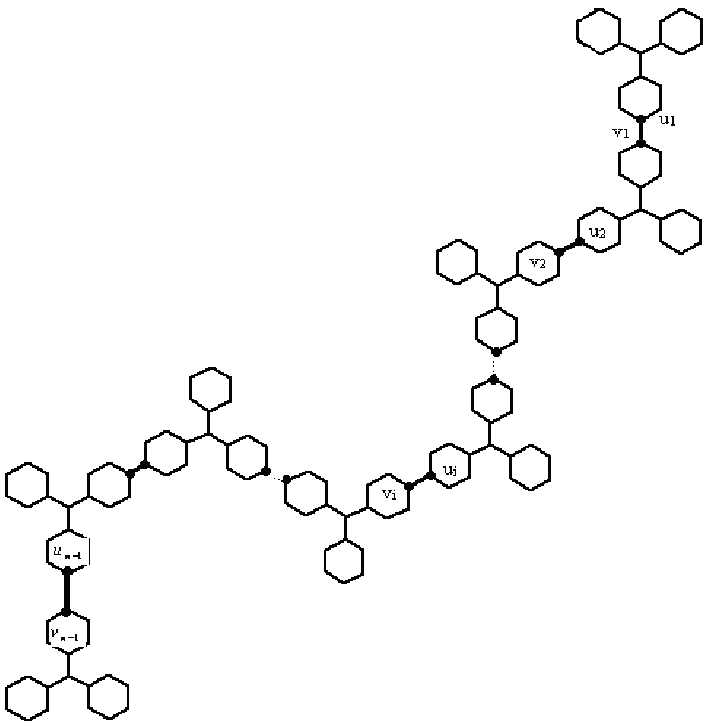

Fig. 3. The chain graph G_n and the labeling of its vertices.

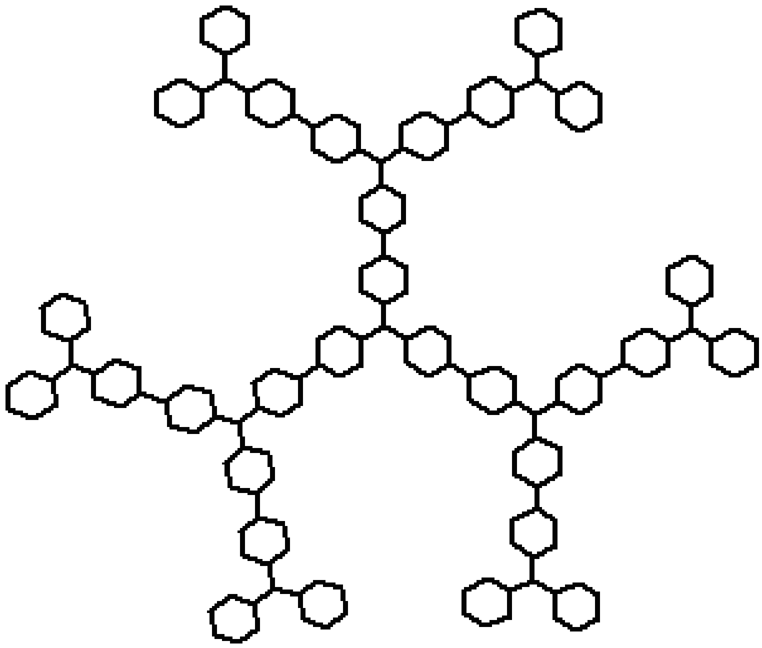

Fig. 4: The graph of the nanostar dendrimer *D*.

REFERENCES

1. H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc.,69 (1947), 17-20.
2. B. Furtula, A. Graovac and D. Vukičević, Atom–bond connectivity index of trees, Disc. Appl. Math., 157 (2009), 2828 - 2835.
3. D. Vukičević and B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, J. Math. Chem., 46 (2009), 1369 – 1376.
4. GH. Fath-Tabar, B. Furtula and I. Gutman, A new geometric--arithmetic index, J. Math. Chem., 47 (2010), 477 – 486.
5. B. Zhou, I. Gutman, B. Furtula and Z. Du, On two types of geometric-arithmetic index, Chem. Phys. Lett., 482 (2009), 153 – 155.
6. M. Ghorbani and A. Khaki, A note on the fourth version of geometric-arithmetic index, Optoelectron. Adv. Mater. – Rapid Comm., 4(12) (2010), 2212-2215.
7. N. Trinajstić and I. Gutman, Mathematical Chemistry, Croat. Chem. Acta, 75 (2002), 329 – 356.
8. A. R. Ashrafi, M. Ghorbani and M. Jalali, Computing Sadhana polynomial of V - phenylenic nanotubes and nanotori, Indian J. Chem., 47 (2008), 535 – 537.
9. A. R. Ashrafi and M. Ghorbani, PI and Omega polynomials of IPR fullerenes, Fullerenes, Nanotubes and Carbon Nanostructures, 18(3) (2010), 198 – 206.

10. A. R. Ashrafi, M. Ghorbani and M. Jalali, Study of IPR fullerenes by counting polynomials, Journal of Theoretical and Computational Chemistry, 8(3) (2009), 451 – 457.
11. A. R. Ashrafi, M. Saheli and M. Ghorbani, The eccentric connectivity index of nanotubes and nanotori, Journal of Computational and Applied Mathematics, 235(16) (2011), 4561-4566.
12. The GAP Team: GAP, Groups, Algorithms and Programming, RWTH, Aachen, 1995.
13. A. R. Ashra i and M. Ghorbani, Eccentric Connectivity Index of Fullerenes, 2008, In: I. Gutman, B. Furtula, Novel Molecular Structure Descriptors – Theory and Applications II, pp. 183 – 192.