

Some topological indices of nanostar dendrimers

M. GHORBANI*, A. MOHAMMADI, F. MADADI

Department of Mathematics, Faculty of Science, Shahid Rajaee, Teacher Training University, Tehran, 16785-136, I. R. Iran

The GA_4 index is a topological index was defined as $GA_4(G) = \sum_{uv \in E} \frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u) + \varepsilon(v)}$, in which eccentricity of vertex u denoted by $\varepsilon(u)$. Recently some classes of GA index were introduced. In this paper we compute the GA_4 index of nanostar dendrimers.

(Received August 12, 2010; accepted November 10, 2010)

Keywords: Topological index, Nanostar dendrimer

1. Introduction

By a graph means a set of vertices and edges which denotes by $V(G)$ and $E(G)$, 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. Throughout this paper graph means simple connected graph.

Molecular descriptors play a prominent map in chemistry, pharmacology, etc. Among them, topological indices are very important [1]. 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. Obviously, the number of vertices and the number of edges are topological index. 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 . For a vertex u of $V(G)$ its eccentricity $\varepsilon(u)$ is the largest distance between u and any other vertex v of G , $\varepsilon(u) = \max_{v \in V(G)} d_G(u, v)$. The maximum eccentricity over all vertices of G is called the diameter of G and denoted by $D(G)$. The eccentric connectivity index [2-6] $\xi(G)$ of a graph G is defined as

$$\xi(G) = \sum_{u \in V(G)} \deg_G(u) \varepsilon(u),$$

where, $\deg_G(u)$ denotes the degree of vertex u in G , $i.e.$, the number of its neighbors in G .

The geometric – arithmetic index (GA) considered by Vukićević and Furtula [7] as

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

Fath-Tabar et al. [8] defined the second version of GA index as follows:

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

where n_u is the number of vertices of G lying closer to the vertex u than to the vertex v . The third member of this class was considered by Zhou et al. [9] as

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

where m_u is the number of edges of G lying closer to the vertex u than to the vertex v . The fourth member of this class was considered by A. R. Ashrafi et al. [10] as

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

in which eccentricity of vertex u denoted by $\varepsilon(u)$. Recently Furtula et al.¹¹ introduced atom-bond connectivity (ABC) index, which it has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows:

$$ABC(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}}.$$

Through this paper our notations are standard and mainly taken from graph theory book such as [12, 13] and [14 - 41].

2. Main results and discussions

In this section, we compute these topological indices for an infinite family of nanostar dendrimers G_n shown in Fig. 1.

Lemma 1. Consider the nanostar dendrimer G_n . Then, for $0 \leq i \leq 9n - 5$ we have

$$\varepsilon(v_i) = 18n - 10 - i.$$

Proof. It is easy to see that the diameter of graph G_1 is 8. This value for G_2 is $3 \times 8 + 2$. By induction one can deduce that the diameter of G_n is $8(2n - 1) + (2n - 2) = 18n - 10$. Since $\varepsilon(v_0) = 18n - 10$, then $\varepsilon(v_1) = 18n - 10 - 1$ and so $\varepsilon(v_i) = 18n - 10 - i$ ($0 \leq i \leq 9n - 5$). Now by using the symmetry of graph the proof is completed.

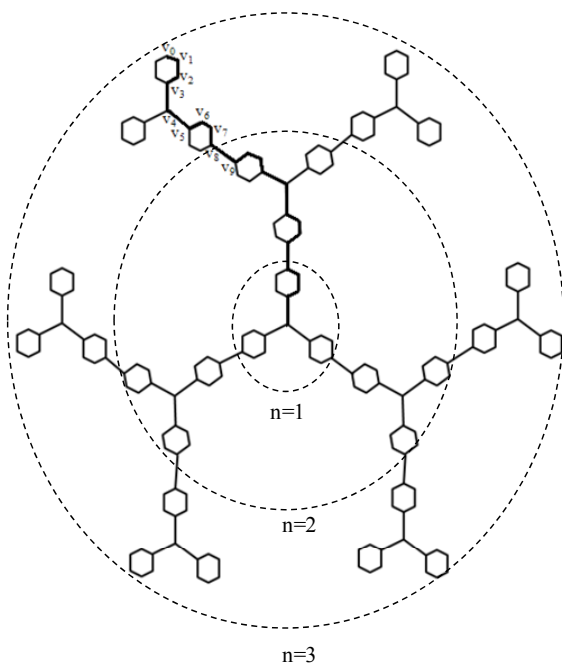


Fig. 1. 2 - D Graph of Nanostar Dendrimer G_n , $n = 3$.

Theorem 2.

$$\xi(G_n) = \sum_{i=0}^{n-2} 3 \times 2^{n-i-2} (6 \sum_{j=0,3} A_{i,j} + 8 \sum_{j=1,2} A_{i,j} + 3 \sum_{j=4,5,8,9} A_{i,j} + 4 \sum_{j=6,7} A_{i,j} - 36n + 20) + 405n - 120$$

where $A_{i,j} = 18n - 10 - 10i - j$.

Theorem 3.

$$GA_4(G_n) = \sum_{i=0}^{n-2} (3 \times 2^{n-i-2}) \left(4 \sum_{j=0}^2 A_{i,j} + 2 \sum_{j=3,5,6,7} A_{i,j} + \sum_{j=4,8} A_{i,j} \right) + 6 \sum_{i=1}^3 \frac{2\sqrt{(9n-i)(9n-i-1)}}{18n-2i-1} + 6 \frac{\sqrt{(9n-4)(9n-5)}}{18n-9}$$

where

$$A_{i,j} = \frac{2\sqrt{(18n-10-9i-j)(18n-11-9i-j)}}{36n-21-18i-2j}.$$

Proof. It should be noted that in the i 'th level of graph G_n there exist $3 \times 2^{i-2}$ copy of G_1 . By substitution values of $\varepsilon(u)$ in Lemma 1 in terms of GA_4 the proof is clear.

Corollary 4.

$$ABC_3(G_n) = \sum_{i=0}^{n-2} (3 \times 2^{n-i-2}) \left(4 \sum_{j=0}^2 A_{i,j} + 2 \sum_{j=3,5,6,7} A_{i,j} + \sum_{j=4,8} A_{i,j} \right) + 6 \sum_{i=1}^3 \frac{\sqrt{18n-2i-3}}{(9n-i)(9n-i-1)} + 3 \frac{\sqrt{18n-11}}{(9n-4)(9n-5)},$$

where

$$A_{i,j} = \frac{\sqrt{36n-23-18i-2j}}{(18n-10-9i-j)(18n-11-9i-j)}.$$

References

- [1] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.
- [2] V. Sharma, R. Goswami, A. K. Madan, J. Chem. Inf. Comput. Sci., **37**, 273 (1997).
- [3] H. Dureja, A. K. Madan, Med. Chem. Res., **16**, 331 (2007).
- [4] V. Kumar, S. Sardana, A. K. Madan, J. Mol. Model., **10**, 399 (2004).
- [5] S. Gupta, M. Singh, A. K. Madan, J. Math. Anal. Appl., **266**, 259 (2002).
- [6] S. Sardana, A. K. Madan, MATCH Commun. Math. Comput. Chem., **43**, 85 (2001).
- [7] D. Vukičević, B. Furtula, J. Math. Chem., **46**, 1369 (2009).
- [8] G. Fath-Tabar, B. Furtula, I. Gutman, J. Math. Chem., in press.
- [9] B. Zhou, I. Gutman, B. Furtula, Z. Du, Chem. Phys. Lett., **482**, 153 (2009).
- [10] A. R. Ashrafi, M. Ghorbani, Optoelectron. Adv. Mater. - Rapid Commun., (Submitted).
- [11] B. Furtula, A. Graovac, D. Vukičević, Disc. Appl. Math., **157**, 2828 (2009).
- [12] N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton, FL (1992).
- [13] D. B. West, Introduction to Graph theory, Prentice Hall, Upper Saddle River, 1996.
- [14] M. Ghorbani, Optoelectron. Adv. Mater. - Rapid Commun., **4**(2), 261, 2010.
- [15] A. R. Ashrafi, M. Saheli, M. Ghorbani, Journal of Computational and Applied Mathematics, <http://dx.doi.org/10.1016/j.cam.2010.03.001>.
- [16] A. R. Ashrafi, H. Saati, M. Ghorbani, Digest Journal of Nanomaterials and Biostructures, **3**(4), 227 (2008).
- [17] A. R. Ashrafi, M. Ghorbani, M. Jalali, Digest Journal of Nanomaterials and Biostructures, **3**(4), 245 (2008).
- [18] M. Ghorbani, M. Jalali, Digest Journal of Nanomaterials and Biostructures, **3**(4), 269 (2008).
- [19] A. R. Ashrafi, M. Ghorbani, Digest Journal of Nanomaterials and Biostructures, **4**(2), 313 (2009).

- [20] A. R. Ashrafi, M. Ghorbani, M. Hemmasi, *Digest Journal of Nanomaterials and Biostructures*, **4**(3), 483 (2009).
- [21] A. R. Ashrafi, M. Ghorbani, *Digest Journal of Nanomaterials and Biostructures*, **4**(2), 389 (2009).
- [22] M. Ghorbani, M. B. Ahmadi, M. Hemmasi, *Digest Journal of Nanomaterials and Biostructures*, **3**(4), 269 (2009).
- [23] M. Ghorbani, M. Jalali, *Digest Journal of Nanomaterials and Biostructures*, **4**(1), 177 (2009).
- [24] M. Ghorbani, M. Jalali, *Digest Journal of Nanomaterials and Biostructures*, **4**(3), 403 (2009).
- [25] A. R. Ashrafi, M. Ghorbani, M. Jalali, *Optoelectron. Adv. Mater. – Rapid Commun.*, **3**(8), 823 (2009).
- [26] A. R. Ashrafi, M. Ghorbani, *Optoelectron. Adv. Mater. – Rapid Commun.*, **3**(6), 596 (2009).
- [27] M. A. Hosseinzadeh, M. Ghorbani, *Optoelectron. Adv. Mater. – Rapid Commun.*, **11**(11), 1671 (2009).
- [28] M. Ghorbani, A. R. Ashrafi, M. Hemmasi, *Optoelectron. Adv. Mater. – Rapid Commun.*, **3**(12), 1306 (2009).
- [29] M. Ghorbani, M. Jalali, *Digest Journal of Nanomaterials and Biostructures*, **4**(4), 681 (2009).
- [30] M. Ghorbani, *Optoelectron. Adv. Mater. – Rapid Commun.*, **4**(2), 261 (2010).
- [31] M. A. Hosseinzadeh, M. Ghorbani, *Optoelectron. Adv. Mater. – Rapid Commun.*, **4**(3), 378 (2010).
- [32] M. Ghorbani, M. Jaddi, *Optoelectron. Adv. Mater. – Rapid Commun.*, **4**(4), 540 (2010).
- [33] H. Maktabi, J. Davoudi, M. Ghorbani, *Optoelectron. Adv. Mater. – Rapid Commun.*, **4**(4), 550 (2010).
- [34] M. Ghorbani, H. Hosseinzadeh, *Optoelectron. Adv. Mater. – Rapid Commun.*, **4**(4), 538 (2010).
- [35] M. Faghani, M. Ghorbani, *MATCH Commun. Math. Comput. Chem.*, **65**, 21 (2010).
- [36] M. Ghorbani, *MATCH Commun. Math. Comput. Chem.*, **65**, 183 (2010).
- [37] M. Ghorbani, M. Ghazi, S. Shakeraneh, *Optoelectron. Adv. Mater. – Rapid Commun.*, **4**(6), 893 (2010).
- [38] M. Ghorbani, M. Ghazi, S. Shakeraneh, *Optoelectron. Adv. Mater. – Rapid Commun.*, **4**(7), 1033 (2010).
- [39] A. Azad, M. Ghorbani, *Optoelectron. Adv. Mater. – Rapid Commun.*, **4**(7), 1261 (2010).
- [40] H. Mesgarani, M. Ghorbani, *Optoelectron. Adv. Mater. – Rapid Commun.*, **4**(7), 1264 (2010).
- [41] M. Ghorbani, A. Azad, M. Ghasemi, *Optoelectron. Adv. Mater. – Rapid Commun.*, **4**(7), 1268 (2010).

*Corresponding author: mghorbani@srttu.edu