Journal of Mathematical Nanoscienese 7 (1) (2017) 23–28

Journal of Mathematical Nanoscience

Available Online at: http://jmathnano.sru.ac.ir

Shahid Rajaee Teacher Training University

The second eccentric Zagreb index of the nanostar dendrimer $D_3[n]$

Mohammad Reza Farahani[1] *, Abdul Qudair Baig[2] , Wasim Sajjad[3]

[1]Department of Applied Mathematics, Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran.

[2]Department of Mathematics, COMSATS Institute of Information Technology, Attock Campus, Pakistan.

[3]Department of Mathematics, University of Sargodha, Mandi Bahauddin Campus, Mandi Bahauddin Pakistan.

Academic Editor: Modjtaba Ghorbani

Abstract. Let $G = (V, E)$ be a simple graph. We denote a vertex by v, where $v \in V(G)$ and edge by e, where $e = uv \in E(G)$. We denote degree of vertex v by d_v which is defined as the number of vertices adjacent with vertex v. The distance between two vertices of G is the length of the shortest path connecting these two vertices which is denoted by $d(u,v)$, where $u,v \in V(G)$. The eccentricity $ecc(v)$ of a vertex v in G is the distance between vertex v and vertex farthest from v in G. In this paper, we consider an infinite family of nanostar dendrimers and we compute its second eccentric Zagreb index. Ghorbani and Hosseinzadeh introduced the second eccentric Zagreb index as $EM_2(G) = \sum_{uv \in E(G)} \left(ecc(u) \times ecc(v)\right)$, that $ecc(u)$ denotes the eccentricity of vertex u and $ecc(v)$ denotes the eccentricity of vertex v of G.

Keywords. molecular graph, eccentricity, Zagreb topological index, nanostar dendrimer, $D_3[n]$.

*Corresponding author (Email address: mrfarahani88@gmail.com).
DOI: 10.22061/JMNS.2017.670

 ©Shahid Rajaee Teacher Training University

1 Introduction

Chemical graph theory is a branch of mathematical chemistry which has an important effect on the development of the chemical sciences. A topological index is a numerical value associated with the chemical constitution of a certain chemical compound aiming to correlate various physical and chemical properties, or some biological activity in it. Carbon nanostructures have found many potential industrial applications such as energy storage, gas sensors, biosensors, nanoelectronic devices and chemical probes [23], just to name a few. Carbon allotropes such as carbon nanocones and carbon nanotubes have been proposed as possible molecular gas storage devices [1,32].

The nanostar dendrimer is a part of a new group of macromolecules that seem like photon funnels just like artificial antennas, and also is a great resistant of photo bleaching. Recently, the mathematical properties of these nanostructures nanostructures have been investigated in [24,29–31].

Let $G = (V,E)$ be a simple connected molecular graph with the vertex and edge set denoted by $V(G)$ and $E(G)$, respectively. Throughout this paper, graph means simple connected graph [17,18,28]. If $x,y \in V(G)$ then the distance $d(u,v)$ between u and v is defined as the length of a minimum path connecting u and v. The eccentricity $ecc(u)$ of a vertex u in G is the largest distance between u and any other vertex of G. The *eccentric connectivity index* of the molecular graph G, was proposed by Sharma, Goswami and Madan [27] as,

$$\xi(G) = \sum_{u \in V(G)} d_v ecc(v),$$

where d_v is the degree of the vertex v and $ecc(v)$ is the eccentricity of the vertex v.

The Zagreb topological indices was introduced by I. Gutman and N. Trinajstić in 1972 [17,18]. The first and second zagreb indices are defined as

$$M_1(G) = \sum_{e=uv \in E(G)} (d_u + d_v),$$

$$M_2(G) = \sum_{e=uv \in E(G)} (d_u \times d_v),$$

where d_v denotes the degree of v. Mathematical properties of the first Zagreb index for general graphs can be found in [17,18,26,28].

In 2012, the *second eccentric Zagreb index* was introduced by Ghorbani and Hosseinzadeh, where the eccentric version of second Zagreb index of the molecular graph G and it is equal to [15]

$$EM_2(G) = \sum_{uv \in E(G)} [ecc(u) \times ecc(v)],$$

where $ecc(u)$ is the eccentricity of the vertex u and $ecc(v)$ is the eccentricity of the vertex v.

In this study, we consider an infinite family of nanostar dendrimers and compute its second eccentric Zagreb index.

2 Results and Discussion

Here, we compute the second eccentric Zagreb index of an infinite family of nanostar dendrimers. We denote the n^{th} growth of nanostar dendrimer for all$n \geq 1$ by $D_3[n]$. From Figure 1, one can see that the general representation of this family of nanostar has $21(2^{n+1}) - 20$ vertices/atoms and $24(2^{n+1} - 1)$ bonds/edges [11–13]. Also, the nanostar dendrimer $D_3[n]$ has a core depicted in Figure 2 and the repeated element cycle C_6 that we named by *leaf*. The n^{th} growth of nanostar dendrimer has

$$\xi_n 3 \sum_{i=0}^{n} (2^i) = 3(\frac{2^{n+1} - 1}{2 - 1}),$$

of leafs, see Figure 2.

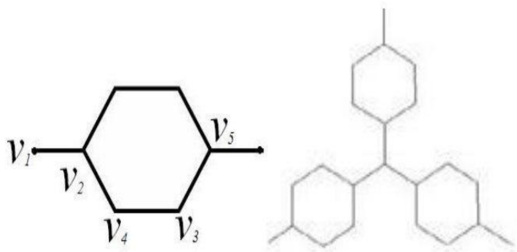

Figure 1. An example of the nanostar dendrimer $D_3[n]$, for $n = 3$ [11–14].

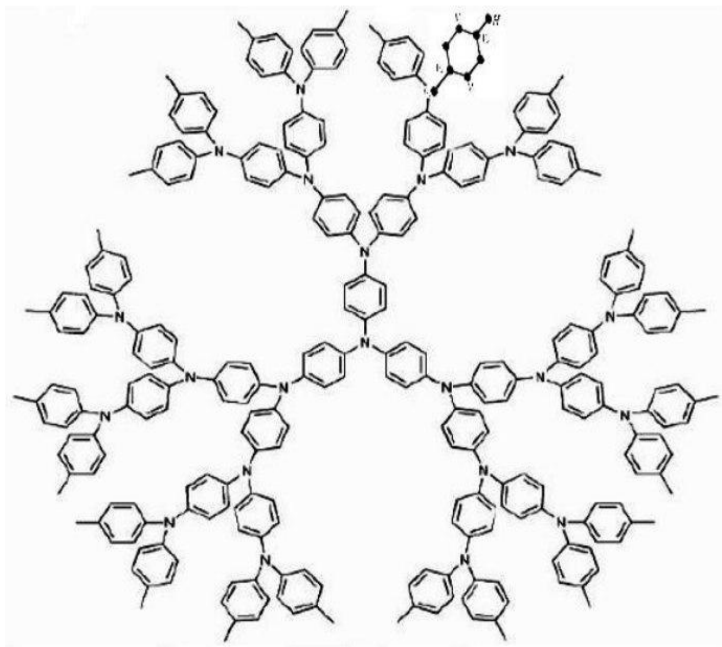

Figure 2. The added graph in each branch and $D_3[0]$ is the primal structure of nanostar dendrimer $D_3[n]$ [11–14].

Consider the $(n-1)^{th}$ growth of nanostar dendrimer in $D_3[n-1]$. We would like to construct $D_3[n]$. In every branch of $D_3[n]$, the leaf graph added. From Figure 2, one can see that the maximum eccentricity of a leaf of $D_3[n]$ is 6 and the eccentricity of previous vertices of core $D_3[0]$ are equal to 10. Thus, for eccentric of vertices in added leaf of nanostar dendrimer $D_3[n-1]$ to $D_3[n]$, we can conclude the following results:

For all $i = 1,2,....,n$, we have $3(2^{i-1})$ vertices of kind labeled $V_1[i]$ with eccentricity $5i + 5(i+1)$ and $3(2^i)$ vertices of kind labeled $V_2[i]$ with eccentricity $5i + 5(i+1)$. Also, there are $3(2^{i+1})$ vertices of $V_3[i]$ and $V_4[i]$, with eccentricies $10i+7$ and $10i+8$, respectively. Morever, for the vertices of $V_5[i]$ have eccentricity of $10i+9$.

Therefore, by using the mentioned results, we have the following computations for third Zagreb index of the n^{th} growth of nanostar dendrimer $D_3[n]$.

Theorem 2.1. *We consider the graph of nanostar dendrimer $D_3[n]$. Then second eccentric Zagreb index is equal to*

$$\begin{aligned} EM_2(D_3[n]) = EM_2(D_3[0]) &+ 3\sum_{\forall i=1,...,n} 2^i(100i^2+110i+30) \\ &+ 6\sum_{\forall i=1,...,n} 2^i(100i^2+130i+42) + 6\sum_{\forall i=1,...,n} 2^i(100i^2+150i+56) \\ &+ 6\sum_{\forall i=1,...,n} 2^i(100i^2+170i+72) + 3(2^n)(100n^2+190n+90). \end{aligned}$$

Proof. Let G be the graph of nanostar dendrimer $D_3[n]$. Hence, we have

$$\begin{aligned} EM_2(D_3[n]) = EM_2(D_3[0]) &+ \sum_{\forall i=1,...,n; uv\in E(D_3[n]) u\in V_1[i], v\in V_2[i]} \big(ecc(u)\times ecc(v)\big) \\ &+ \sum_{\forall i=1,...,n; uv\in E(D_3[n]) u\in V_2[i], v\in V_3[i]} \big(ecc(u)\times ecc(v)\big) \\ &+ \sum_{\forall i=1,...,n; uv\in E(D_3[n]) u\in V_3[i], v\in V_4[i]} \big(ecc(u)\times ecc(v)\big) \\ &+ \sum_{\forall i=1,...,n; uv\in E(D_3[n]) u\in V_4[i], v\in V_5[i]} \big(ecc(u)\times ecc(v)\big) \\ &+ \sum_{vH\in(D_3[n]), H\in V_1[n+1], v\in V_5[n]} \big(ecc(H)\times ecc(v)\big), \end{aligned}$$

$$\begin{aligned} EM_2(D_3[n]) = EM_2(D_3[0]) &+ \sum_{\forall i=1,...,n} 3(2^i)\big(ecc(V_1[i])\times ecc(V_2[i])\big) \\ &+ \sum_{\forall i=1,...,n} 3(2^i)\big(ecc(V_2[i])\times ecc(V_3[i])\big) \\ &+ \sum_{\forall i=1,...,n} 3(2^i)\big(ecc(V_3[i])\times ecc(V_4[i])\big) \\ &+ \sum_{\forall i=1,...,n} 3(2^i)\big(ecc(V_4[i])\times ecc(V_5[i])\big) \\ &+ 3(2^n)\big(ecc(H)\times ecc(V_5[n])\big). \end{aligned}$$

By using above values we get

$$\begin{aligned} EM_2(D_3[n]) = EM_2(D_3[0]) &+ \sum_{\forall i=1,\ldots,n} 3(2^i)\big((10i+5)\times(10i+6)\big) \\ &+ \sum_{\forall i=1,\ldots,n} 3(2^{i+1})\big((10i+6)\times(10i+7)\big) \\ &+ \sum_{\forall i=1,\ldots,n} 3(2^{i+1})\big((10i+7)\times(10i+8)\big) \\ &+ \sum_{\forall i=1,\ldots,n} 3(2^{i+1})\big((10i+8)\times(10i+9)\big) \\ &+ 3(2^n)\big((10n+10)\times(10n+9)\big). \end{aligned}$$

After doing some calculations, we have

$$\begin{aligned} EM_2(D_3[n]) = EM_2(D_3[0]) &+ 3\sum_{\forall i=1,\ldots,n} 2^i(100i^2+110i+30) \\ &+ 6\sum_{\forall i=1,\ldots,n} 2^i(100i^2+130i+42) + 6\sum_{\forall i=1,\ldots,n} 2^i(100i^2+150i+56) \\ &+ 6\sum_{\forall i=1,\ldots,n} 2^i(100i^2+170i+72) + 3(2^n)(100n^2+190n+90). \end{aligned}$$

□

3 Conclusion

In this paper, we examined the eccentric connectivity index, first Zagreb index and second Zagreb index. We have considered an infinite family of nanostar dendrimers and we computed its second eccentric Zagreb index.

References

[1] O. Adisa, B. J. Cox and J. M. Hill, Modelling the surface adsorption of methane on carbon nanostructures, Carbon 49 (10) (2011) 3212–3218.

[2] A. R. Ashrafi and M. Mirzargar, PI Szeged, and edge Szeged indices of an infinite family of nanostar dendrimers, Indian J. Chem. 47A (2008) 538–541.

[3] A. R. Ashrafi and P. Nikzad, Connectivity index of the family of dendrimer nanostars, Digest. J. Nanomater. Bios. 4 (2) (2009) 269–273.

[4] A. R. Ashrafi and P. Nikzad, Kekule index and bounds of energy for nanostar dendrimers, Digest. J. Nanomater. Bios. 4 (2) (2009) 383–388.

[5] S. Alikhani and M. A. Iranmanesh, Chromatic polynomials of some dendrimers, MATCH Commun. Math. Comput. Chem. 62 (2009) 363–370.

[6] S. Alikhani and M. A. Iranmanesh, Chromatic polynomials of some dendrimers, J. Comput. Theor. Nanosci. 7 (11) (2010) 2314–2316.

[7] S. Alikhani and M. A. Iranmanesh, Chromatic polynomials of some nanostars, Iranian Journal of Math. Chemist. 3 (2) (2010) 127–135.

[8] S. Alikhani and M. A. Iranmanesh, Eccentric connectivity polynomials of an infinite family of dendrimers, Digest. J. Nanomater. Bios. 6 (1) (2011) 256–257.

[9] G. Chartrand and P. Zhang, Introduction to Graph Theory, Tata Mcgraw-Hill Edition.

[10] M. Eliasi and B. Taeri, Szeged index of armchair polyhex nanotubes, MATCH Commun. Math. Comput. Chem. 59 (2008) 437–450.

[11] M. R. Farahani, Fourth atom-bond connectivity index of an infinite class of nanostar dendrimer $D_3[n]$, Journal of Advances in Chemistry 4 (1) (2013) 301–305.

[12] M. R. Farahani, Computing fifth geometric-arithmetic index of dendrimer nanostars, Advances in Materials and Corrosion 1 (2013) 62–64.

[13] M. R. Farahani, Some connectivity index of an infinite class of dendrimer nanostars, Journal of Applied Physical Science International 3 (3) (2015) 99–105.

[14] M. R. Farahani, The second Zagreb eccentricity index of polycyclic aromatic hydrocarbons PAH_K, Journal of Computational Methods in Molecular Design 5 (2) (2015) 115–120.

[15] M. Ghorbani and M. A. Hosseinzadeh, A new version of Zagreb indices, Filomat 26 (1) (2012) 93–100.

[16] M. Golriz, M. R. Darafsheh and M.H. Khalifeh, The Wiener, Szeged and PI-indices of a phenylazomethine dendrimer, Digest. J. Nanomater. Bios. 6 (4) (2011) 1545–1549.

[17] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. III. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972) 535–538.

[18] I. Gutman and K. C. Das, The first Zagreb index 30 years after, MATCH Commun. Math. Comput. Chem. 50 (2004) 83–92.

[19] Y. Gao, W. Gao and L. Liang, Certain general Zagreb indices and Zagreb polynomials of molecular graphs, International Journal of Chemical and Biomolecular Science 1 (1) (2015)1–5.

[20] A. Heydari and B. Taeri, Szeged index of armchair polyhex nanotubes, MATCH Commun. Math. Comput. Chem (2007) 57–463.

[21] N. M. Husin, R. Hasni and N. E. Arif, Atom-bond connectivity and geometric-arithmetic indices of dendrimer nanostars, Australian Journal of Basic and Applied Sciences 7(9) (2013) 10–14.

[22] A. Karbasioun and A. R. Ashrafi, Wiener and detour indices of a new type of nanostar dendrimers, Macedonian journal of chemistry and chemical engineering 28 (1) (2009) 49–54.

[23] S. Iijima, Helical microtubules of graphitic carbon, Nature 354 (1991) 56–58. doi:10.1038/354056a0

[24] X. Li and Y. Shi, A survey on the Randic index, MATCH Commun. Math. Comput. Chem. 59 (1) (2008) 127–156.

[25] G. R. Newkome, C. N. Moorefield and F. Vögtle, Dendrimer and dendrons, concepts, syntheses, applications, Vol. 623. Weinheim: Wiley-vch, (2001).

[26] S. Nikolić, G. Kovačević, A. Miličević and N. Trinajstić, The Zagreb indices 30 years after, Croat. Chem. Acta. 76 (2003) 113–124.

[27] V. Sharma, R. Goswami and A. K. Madan, Eccentric connectivity index, A novel highly discriminating topological descriptor for structure-property and structure-activity studies, J. Chem. Inf. Comput. Sci. 37 (1997) 273–282.

[28] R. Todeschini and V. Consonni, Handbook of molecular descriptors, Wiley-VCH, Weinheim, (2000). doi:10.1002/9783527613106

[29] D. Vukiccevic 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.

[30] S. Wang and B. Wei, Multiplicative Zagreb indices of k-trees, Discrete Appl. Math. 180 (2015) 168–175.

[31] Y. Zhai, J. B. Liu and S. Wang, Structure properties of Koch networks based on networks dynamical systems, Complexity (2017).

[32] J. Zhao, A. Buldum, J. Han and J. P. Lu, Gas molecule adsorption in carbon nanotubes and nanotube bundles, Nanotechnology 13 (2002) 195–200.