STUDIA UBB CHEMIA, LXI, 1, 2016 (p. 127-140)
(RECOMMENDED CITATION)

Dedicated to Professor Mircea Diudea on the Occasion of His 65th Anniversary

THEORETICAL STUDY OF NANOSTAR DENDRIMERS

NAJMEH SOLEIMANI[a,*], ESMAEEL MOHSENI[b], SAHAR HELALBIN[b]

ABSTRACT. In this paper, we give some theoretical results about nanostar dendrimers by topological indices. Formulas for computing topological indices based on distance and degree in a graph such as eccentric connectivity, total eccentricity, fourth version of atom-bond connectivity and fifth version of geometric-arithmetic indices of two types of nanostar dendrimers are presented.

Keywords: *Dendrimers, Eccentric, Vertex-degree, Connectivity indices.*

INTRODUCTION

Dendrimers are large and complex molecules with well taylored chemical structures. There are numerous topological descriptors that have found applications in theoretical chemistry, particularly in QSPR/QSAR research [1]. Among them, topological indices have a prominent place. In some research papers [2-9], the authors have computed some topological indices of nanostar dendrimers, nanostructures and other graphs.

In this paper, we discuss four topological descriptors, namely ξ^c, θ, ABC_4 and GA_5 indices for two types of nanostar dendrimers. The article is organized as follows: whitin the second part of this work, we give the necessary definitions. Section 3 contains our main results. Conclusions and references will close this article.

[a] *Young Researchers and Elite Club, Qaemshahr Branch, Islamic Azad University, Qaemshahr, Iran*
[b] *Salehan Institute of Higher Education, Qaemshahr, Iran*
[*] *Corresponding Author: soleimani.najmeh@gmail.com*

DEFINITIONS

Now, we introduce some notations and terminology which is needed for the rest of the paper. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds of a molecule. Let $G = (V, E)$ be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge sets of it are represented by $V = V(G)$ and $E = E(G)$, respectively. The degree (i.e., the number of first neighbors) of a vertex $u \in V(G)$ is denoted by $deg_G(u)$. The edge connecting the vertices u and v is denoted by uv. The distance between u and v in $V(G)$, $d(u, v)$, is the length of a shortest u_v path in G. For a vertex u of $V(G)$ its eccentricity $\varepsilon_G(u)$ is the largest distance between u and any other vertex v of G, $\varepsilon_G(u) = max\{d(u, v)|\ v \in V(G)\}$. The maximum and minimum eccentricity over all vertices of G are called the diameter and radius of G and denoted by $d(G), r(G)$ respectively. In 2011, Doslić et al. [10], have proposed the eccentric connectivity polynomial. This polynomial is defined as follows:

$$\xi^c(G, x) = \sum_{u \in V(G)} deg_G(u) x^{\varepsilon_G(u)},$$

where x is a dummy variable. A topological index is a real number derived from molecular graphs of chemical compounds. The oldest topological index is the Wiener index, introduced by Harold Wiener [11]. The eccentric-connectivity index of the molecular graph G, $\xi^c(G)$, was proposed by Sharma et al. [12]. It is easy to see that the eccentric-connectivity index of a graph can be obtained from the corresponding polynomials by evaluating its first derivative, at $x = 1$. The eccentric and total connectivity indices of G are defined as follows:

$$\xi^c(G) = \sum_{u \in V(G)} \deg_G(u) \varepsilon_G(u), \qquad \theta(G) = \sum_{u \in V(G)} \varepsilon_G(u).$$

We encourage readers to references [13–15] to study some properties of eccentric-connectivity index of some nanostructures.

Among topological connectivity indices, the atom-bond connectivity (ABC) index and geometric-arithmetic (GA) index are of great importance. For other studies on these topological indices, we suggest refs. [16,17]. In 2010, Ghorbani et al. [18] introduced a new version of atom-bond connectivity (ABC_4) index. It is defined as follows:

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}},$$

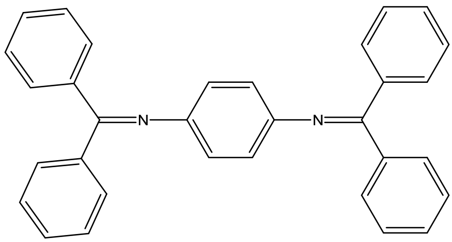
where S_u is the sum of degrees of all vertices adjacent to vertex u. In other words, $S_u = \sum_{v \in N_G(u)} \deg_G(v)$ and $N_G(u) = \{v \in V(G) | uv \in E(G)\}$.

Recently a fifth version of geometric-arithmetic (GA_5) index is proposed by Graovac et al. [19] in 2011, as follows:

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}.$$

RESULTS AND DISCUSSION

The main aim of this section is to compute the eccentric-connectivity polynomial, eccentric-connectivity, total eccentricity, fourth version of atom-bond connectivity and fifth version of geometric-arithmetic indices of the molecular graph of two types of nanostar dendrimers (see Figure 1). In this paper, $D_1[n]$ and $D_2[n]$ denotes the n^{th} growth of nanostar dendrimer for every infinite integer n. For background materials, *see references* [20, 21].



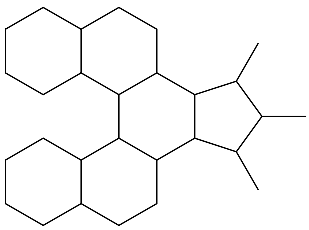


Figure 1. First generation of diphenylazomethine dendrimer (left) and Wang's Helicene-based dendrimers (right).

Calculation of polynomials and topological Indices

Before we proceed to our main results, we explain the examples which will be further used.

Example 1. Let us consider the first kind of nanostar dendrimer, of which grown $1-3$ steps are denoted by $D_1[n]$ for $n = 1, 2, 3$.

Obviously, for $n = 1$, $|V| = 34$ and $|E| = 38$. The eccentric-connectivity polynomial is equal to:

$$\xi^c(D_1[1], x) = 8x^{15} + 16x^{14} + 16x^{13} + 12x^{12} + 6x^{11} + 4x^{10} + 6x^9 + 8x^8.$$

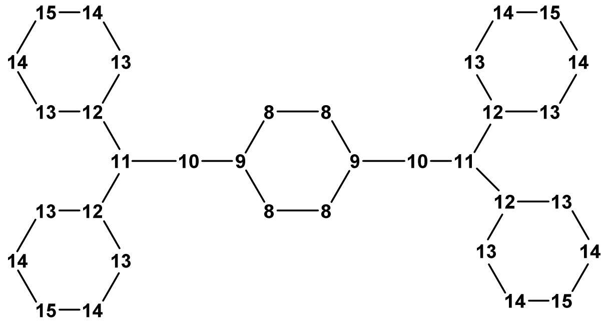


Figure 2. The molecular graph of $D_1[n]$ for $n = 1$.

For $n = 2$, $|V| = 90$ and $|E| = 102$. The eccentric-connectivity polynomial is equal to:

$$\xi^c(D_1[2], x) = 16x^{27} + 32x^{26} + 32x^{25} + 24x^{24} + 12x^{23} + 8x^{22} + 12x^{21} + 16x^{20} + 16x^{19} + 12x^{18} + 6x^{17} + 4x^{16} + 6x^{15} + 8x^{14}.$$

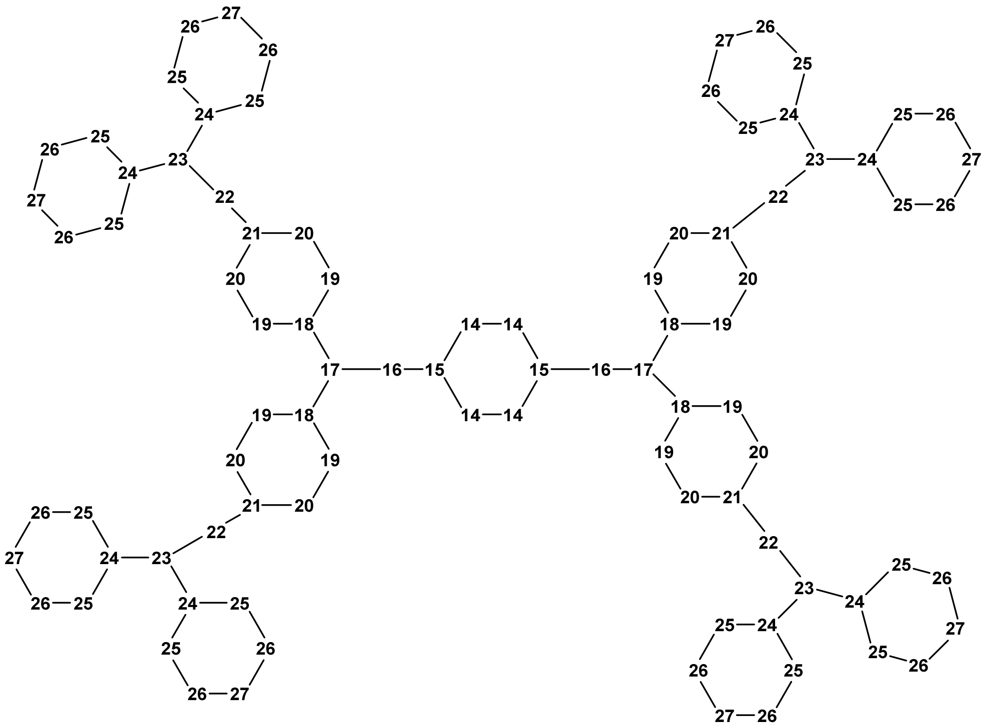


Figure 3. The molecular graph of $D_1[n]$ for $n = 2$.

Also, for $n = 3$, $|\mathrm{V}| = 202$ and $|\mathrm{E}| = 230$. The eccentric-connectivity polynomial is equal to:

$$\xi^c(D_1[3],x) = 32x^{39} + 64x^{38} + 64x^{37} + 48x^{36} + 24x^{35} + 16x^{34} + 24x^{33} + 32x^{32} + 32x^{31} + 24x^{30} + 12x^{29} + 8x^{28} + 12x^{27} + 16x^{26} + 16x^{25} + 12x^{24} + 6x^{23} + 4x^{22} + 6x^{21} + 8x^{20}.$$

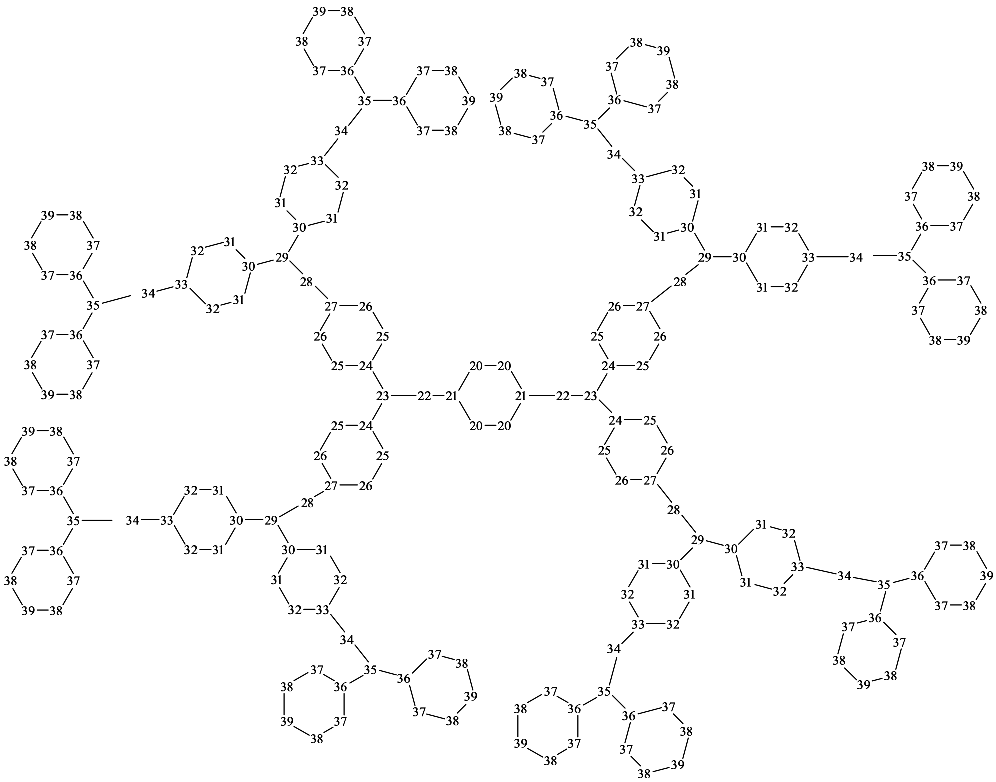


Figure 4. The molecular graph of $D_1[n]$ for $n = 3$.

Using calculations given above, it is possible to evaluate the eccentric-connectivity polynomial of this class of nanostar dendrimers.

Theorem 2. The eccentric-connectivity polynomial of the nanostar dendrimer $D_1[n]$ for $n \geq 1$ is given by the formula:

$$\xi^c(D_1[n],x) = 2^{n+2}\,x^{12n+3} + 2^{n+3}\,x^{12n+2} + \sum_{k=1}^{n} 2^k(8x^{6(n+k)+1} + 6x^{6(n+k)} + 3x^{6(n+k)-1} + 2x^{6(n+k)-2} + 3x^{6(n+k)-3} + 4x^{6(n+k)-4}).$$

Proof. To prove the theorem, we apply induction on n. By considering the general form of this graph, $|V(D_1[n])| = 28 \times 2^n - 22$ and $|E(D_1[n])| = 32 \times 2^n - 26$. We compute maximum vertex eccentric connectivity and minimum vertex eccentric connectivity for nanostar dendrimer graph $D_1[n]$. For $u \in V(D_1[n])$, we have $d(D_1[n]) = 12n + 3$ and $r(D_1[n]) = 6n + 2$. The degrees, frequencies and eccentricities of these vertices are listed in Table 1.

Table 1. The representatives of vertices of $D_1[n]$ with their degree, eccentricity and frequency of occurrence, for $1 \leq k \leq n$.

Vertex type	Degree	Eccentricity	Frequency
1	2	$12n + 3$	2^{n+1}
2	2	$12n + 2$	2^{n+2}
3	2	$6n + 6k + 1$	2^{k+2}
4	3	$6n + 6k$	2^{k+1}
5	3	$6n + 6k - 1$	2^k
6	2	$6n + 6k - 2$	2^k
7	3	$6n + 6k - 3$	2^k
8	2	$6n + 6k - 4$	2^{k+1}

By using data in Table 1 and definition of eccentric-connectivity polynomial calculation may be achieved.

From Theorem 2, it is possible to calculate the eccentric-connectivity index of these nanostar dendrimers. We have:

Theorem 3. The eccentric-connectivity index of $D_1[n]$ for $n \geq 1$ is computed as follows:

$$\xi^c(D_1[n]) = 2^n(768n - 332) - 312n + 360.$$

Proof. From the definition, we have $\xi^c(D_1[n]) = \frac{\partial(\xi^c(D_1[n],x))}{\partial x}|_{x=1}$. Thus:

$$\begin{aligned}\xi^c(D_1[n]) &= 2^{n+2}(12n+3) + 2^{n+3}(12n+2) \\ &+ \sum_{k=1}^{n} 2^k \Big(\big(8(6(n+k)+1)\big) + 6(6(n+k)) + \big(3(6(n+k)-1)\big) \\ &+ \big(2(6(n+k)-2)\big) + \big(3(6(n+k)-3)\big) + \big(4(6(n+k)-4)\big)\Big) \\ &= 2^n(768n - 332) - 312n + 360.\end{aligned}$$

Theorem 4. The total eccentricity index of $D_1[n]$ for $n \geq 1$ is computed as follows:

$$\theta(D_1[n]) = 2^n(336n - 138) - 132n + 152.$$

Proof. The total eccentricity index of a graph is the sum of eccentricities of all the vertices. Therefore by the calculations given in Table 1, the theorem is proved.

Theorem 5. The fourth atom-bond connectivity index of $D_1[n]$ for $n \geq 1$ is computed as follows:

$$ABC_4(D_1[n]) = \frac{4355257157954373 \times 2^{n+2}}{1125899906842624} + \frac{4625405229014641 \times 2^{n}}{2251799813685248} - \frac{3896323959238067}{281474976710656}.$$

Proof. Let $D_1[n]$ be the graph of first kind of nanostar dendrimer. We compute the edge partition of $D_1[n]$ based on the degree sum of neighbors of end vertices of each edge (Table 2).

Table 2. The edge partition of $D_1[n]$ based on the degree sum of neighbors of the end vertices of each edge.

(S_u, S_v) $uv \in E(D_1[n])$	No. edges	(S_u, S_v) $uv \in E(D_1[n])$	No. edges
(4,4)	2^{n+2}	(8,6)	$2^{n+1} - 2$
(5,4)	2^{n+2}	(6,6)	$2^{n+1} - 2$
(7,5)	$2^{n+3} - 8$	(6,5)	$2^{n+2} - 4$
(7,8)	$2^{n+2} - 4$	(5,5)	$2^{n+2} - 6$

Now, we use this partition to compute ABC_4 index of $D_1[n]$.

$$ABC_4(D_1[n]) = \sum_{uv \in E(D_1[n])} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}$$

$$= 2^{n+2}\sqrt{\frac{4+4-2}{4 \times 4}} + 2^{n+2}\sqrt{\frac{5+4-2}{5 \times 4}} + (2^{n+3} - 8)\sqrt{\frac{7+5-2}{7 \times 5}}$$

$$+(2^{n+2} - 4)\sqrt{\frac{7+8-2}{7 \times 8}}$$

$$+(2^{n+1} - 2)\sqrt{\frac{8+6-2}{8 \times 6}} + (2^{n+1} - 2)\sqrt{\frac{6+6-2}{6 \times 6}} + (2^{n+2} - 4)\sqrt{\frac{6+5-2}{6 \times 5}}$$

$$+(2^{n+2} - 6)\sqrt{\frac{5+5-2}{5 \times 5}}.$$

After an easy simplification, we get

$$ABC_4(D_1[n]) = 2^{n+2}\left(\frac{\sqrt{35}+\sqrt{30}+4\sqrt{2}}{10}+\frac{14\sqrt{6}+16\sqrt{14}+\sqrt{728}}{56}\right)+2^n\left(\frac{3+\sqrt{10}}{3}\right)$$
$$-\left(\frac{6+2\sqrt{10}}{6}+\frac{4\sqrt{30}+24\sqrt{2}}{10}+\frac{\sqrt{728}+16\sqrt{14}}{14}\right)$$
$$=\frac{4355257157954373\times 2^{n+2}}{1125899906842624}+\frac{4625405229014641\times 2^n}{2251799813685248}$$
$$-\frac{3896323959238067}{281474976710656},$$

which proves the theorem.

Theorem 6. The fifth geometric-arithmetic index of $D_1[n]$ for $n \geq 1$ is computed as follows:

$$GA_5(D_1[n]) = \frac{2238947875180617\times 2^{n+2}}{281474976710656}-\frac{3636956611970403}{140737488355328}.$$

Proof. By using definition of GA_5 index and Table 2, one can see that:

$$GA_5(D_1[n]) = \sum_{uv\in E(D_1[n])}\frac{2\sqrt{S_uS_v}}{S_u+S_v}$$
$$= 2^{n+2}\frac{2\sqrt{4\times4}}{4+4}+2^{n+2}\frac{2\sqrt{5\times4}}{5+4}+(2^{n+3}-8)\frac{2\sqrt{7\times5}}{7+5}+(2^{n+2}-4)\frac{2\sqrt{7\times8}}{7+8}$$
$$+(2^{n+1}-2)\frac{2\sqrt{8\times6}}{8+6}+(2^{n+1}-2)\frac{2\sqrt{6\times6}}{6+6}+(2^{n+2}-4)\frac{2\sqrt{6\times5}}{6+5}+(2^{n+2}-6)\frac{2\sqrt{5\times5}}{5+5}.$$

After a bit calculation, we get

$$GA_5(D_1[n]) = 2^{n+2}\left(\frac{4\sqrt{5}+3\sqrt{35}}{9}+\frac{75+8\sqrt{14}}{30}+\frac{22\sqrt{3}+14\sqrt{30}}{77}\right)$$
$$-\left(\frac{120+20\sqrt{35}+16\sqrt{14}}{15}+\frac{88\sqrt{3}+56\sqrt{30}}{77}\right)$$
$$=\frac{2238947875180617\times 2^{n+2}}{281474976710656}-\frac{3636956611970403}{140737488355328},$$

that proves our theorem.

Example 7. We consider now the second kind of nanostar dendrimer, with the grown $1-3$ steps denoted by $D_2[n]$ for $n = 1, 2, 3$.

Obviously, for $n = 1$, $|V| = 28$ and $|E| = 33$. The eccentric-connectivity polynomial is equal to:

$$\xi^c(D_2[1], x) = 7x^9 + 21x^8 + 20x^7 + 12x^6 + 6x^5.$$

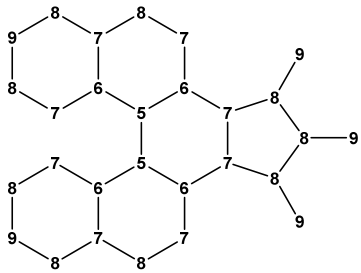


Figure 5. The molecular graph of $D_2[n]$ for $n = 1$.

For $n = 2$, $|V| = 82$ and $|E| = 99$. The eccentric-connectivity polynomial is equal to:

$$\xi^c(D_2[2], x) = 8x^{27} + 16x^{26} + 20x^{25} + 20x^{24} + 20x^{23} + 12x^{22} + 16x^{21}$$
$$+12x^{20} + 6x^{19} + 9x^{18} + 21x^{17} + 20x^{16} + 12x^{15} + 6x^{14}.$$

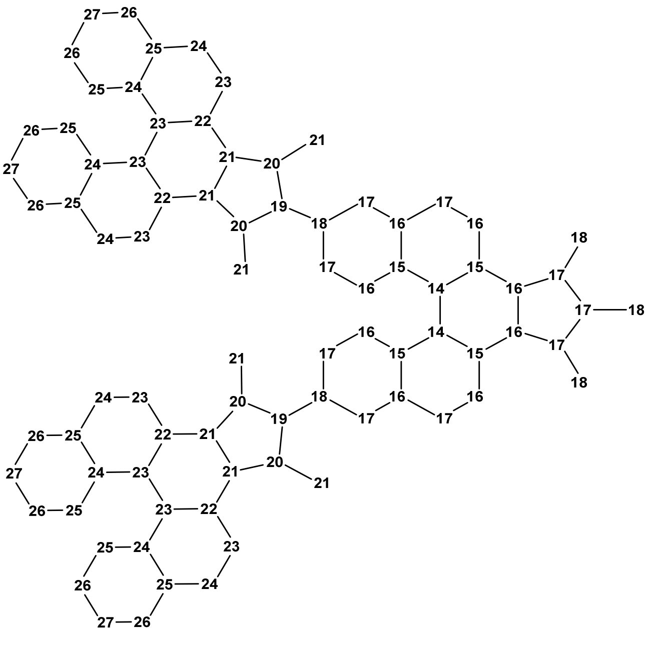


Figure 6. The molecular graph of $D_2[n]$ for $n = 2$.

Also, for $n = 3$, $|V| = 190$ and $|E| = 231$. The eccentric-connectivity polynomial is equal to:

$$\xi^c(D_2[3], x) = 16x^{45} + 32x^{44} + 40x^{43} + 40x^{42} + 40x^{41} + 24x^{40} + 32x^{39} + 24x^{38} + 12x^{37} + 12x^{36} + 16x^{35} + 20x^{34} + 20x^{33} + 20x^{32} + 12x^{31} + 16x^{30} + 12x^{29} + 6x^{28} + 9x^{27} + 21x^{26} + 20x^{25} + 12x^{24} + 6x^{23}.$$

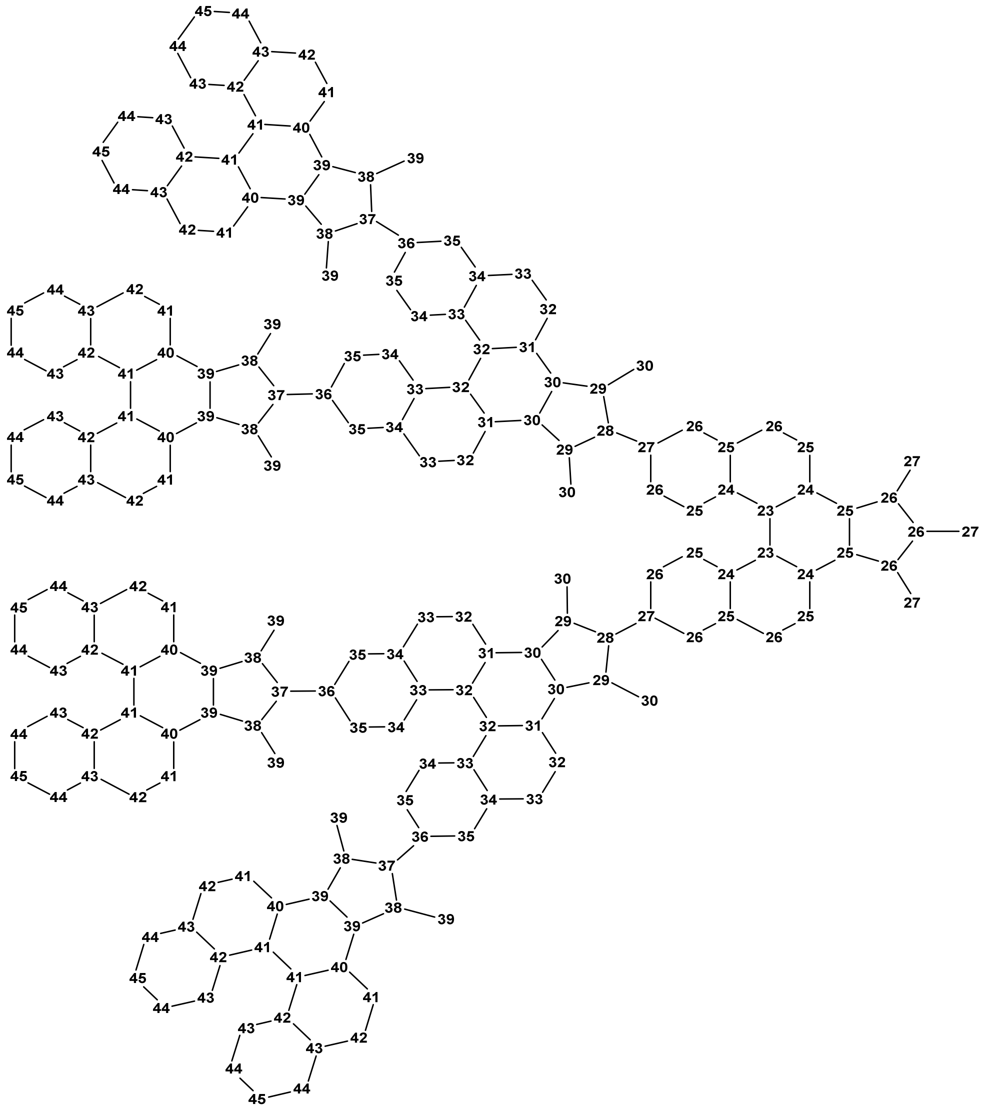


Figure 7. The molecular graph of $D_2[n]$ for $n = 3$.

Similar to the proof of Theorem 2, we can prove the following theorem:

Theorem 8. The eccentric-connectivity polynomial of the nanostar dendrimer $D_2[n]$ for $n \geq 3$ is computed as follows:

$$\xi^c(D_2[n],x) = 2^{n+1}x^{18n-9} + 9x^{9n} + 21x^{9n-1} + 20x^{9n-2} + 12x^{9n-3} + 6x^{9n-4}$$
$$+ \sum_{k=1}^{n-1} 2^k(8x^{9(n+k)-1} + 10x^{9(n+k)-2} + 10x^{9(n+k)-3} + 10x^{9(n+k)-4}$$
$$+ 6x^{9(n+k)-5} + 8x^{9(n+k)-6} + 6x^{9(n+k)-7} + 3x^{9(n+k)-8})$$
$$+ \sum_{k=1}^{n-2} 2^k(6x^{9(n+k)})$$

Proof. Using a simple calculation, one can show that $|V(D_2[n])| = 27 \times 2^n - 26$ and $|E(D_2[n])| = 33 \times 2^n - 33$. For $u \in V(D_2[n])$, we have $d(D_2[n]) = 18n - 9$ and $r(D_2[n]) = 9n - 4$. By considering the general form of this second nanostar dendrimer, we can fill the Table 3. By using data in this table the proof is straightforward.

Table 3. The representatives of vertices of $D_2[n]$ with their degre, eccentricity and frequency of occurrence, for $1 \leq k \leq n-1$ and $n \geq 3$.

Vertex type	Degree	Eccentricity	Frequency
1	2	$18n-9$	2^n
2	3	$9n$	2
3	1	$9n$	3
4	3	$9n-1$	3
5	2	$9n-1$	6
6	3	$9n-2$	4
7	2	$9n-2$	4
8	3	$9n-3$	4
9	3	$9n-4$	2
10	2	$9n+9k-1$	2^{k+2}
11	3	$9n+9k-2$	2^{k+1}
12	2	$9n+9k-2$	2^{k+1}
13	3	$9n+9k-3$	2^{k+1}
14	2	$9n+9k-3$	2^{k+1}
15	3	$9n+9k-4$	2^{k+1}
16	2	$9n+9k-4$	2^{k+1}
17	3	$9n+9k-5$	2^{k+1}

Vertex type	Degree	Eccentricity	Frequency
18	3	$9n+9k-6$	2^{k+1}
19	1	$9n+9k-6$	2^{k+1}
20	3	$9n+9k-7$	2^{k+1}
21	3	$9n+9k-8$	2^{k}
22	3	$\sum_{k=1}^{n-2} 9n+9k$	$\sum_{k=1}^{n-2} 2^{k+1}$

By Table 3 and some simple calculations by MATLAB, we can prove the following theorem:

Theorem 9. The eccentric-connectivity index and total eccentricity index of $D_2[n]$ for $n \geq 1$ are computed as follows:

$$\xi^c(D_2[n]) = 2^n(1188n - 1439) - 594n + 1569,$$
$$\theta(D_2[n]) = 2^n(486n - 582) - 234n + 633.$$

Theorem 10. The fourth atom-bond connectivity index and fifth geometric-arithmetic index of $D_2[n]$ for $n \geq 1$ are computed as:

$$GA_5(D_2[n]) = \frac{286724064989901 \times 2^n}{8796093022208} - \frac{2298465931078229}{70368744177664}.$$
$$ABC_4(D_2[n]) = \frac{2\sqrt{2}(3\times 2^n - 4)}{5} + \frac{1072236973249725\times 2^n}{70368744177664} - \frac{251086321269759}{17592186044416}.$$

Proof. These results are proven like Theorem 5 and Theorem 6 therefore, we omit the proofs.

Table 4. The edge partition of $D_2[n]$ based on the degree sum of neighbors of the end vertices of each edge.

(S_u, S_v) $uv \in E(D_2[n])$	No. edges	(S_u, S_v) $uv \in E(D_2[n])$	No. edges
(3,7)	$2^{n+1}-1$	(5,5)	$3\times 2^n - 4$
(7,7)	2	(5,7)	$4(2^n-1)$
(7,9)	$5(2^n)-8$	(4,5)	2^{n+1}
(9,9)	$2^{n+1}-2$	(4,4)	2^n
(9,8)	$6(2^n-1)$	(7,8)	$2^{n+1}-2$
(8,5)	$4(2^n-1)$	(6,7)	$4(2^{n-1}-1)$

CONCLUSIONS

Among topological descriptors, topological indices are very important and they play a prominent role in Mathematical Chemistry. In this paper, we studied the nanostar dendrimers. As main results, we derived exact formulas for the eccentric-connectivity index, total eccentricity index, fourth version of atom-bond connectivity index and fifth version of geometric-arithmetic index of two types of nanostar dendrimers.

REFERENCES

1. R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Weinheim, Wiley-VCH, **2000**.
2. N.E. Arif, R. Hasni, S. Alikhani, *Journal of Applied Sciences*, **2012**, *12*, 2279.
3. A.R. Ashrafi, M. Mirzagar, *Indian Journal of Chemistry*, **2008**, *47A*, 538.
4. M.R. Farahani, W. Gao, R. Kanna M.R., *Indian Journal of Fundamental and Applied Life Sciences*, **2015**, *5* (S4), 766.
5. N. Soleimani, M.J. Nikmehr, H.A. Tavallaee, *Studia UBB. Chemia*, **2014**, *59*(4), 139.
6. N. Soleimani, M.J. Nikmehr, H.A. Tavallaee, *Journal of the National Science Foundation of Sri Lanka*, **2015**, *43*(2), 127.
7. M.J. Nikmehr, M. Veylaki, N. Soleimani, *Optoelectron. Adv. Mater.-Rapid Comm.,* **2015**, *9*(9), 1147.
8. M.J. Nikmehr, N. Soleimani, H.A. Tavallaee, *Proceedings of the Institute of Applied Mathematics*, **2015**, *4*(1), 20.
9. M.J. Nikmehr, L. Heidarzadeh, N. Soleimani, *Studia Scientiarum Mathematicarum Hungarica*, **2014**, 51, 133.
10. T. Doslić, M. Ghorbani, M.A. Hosseinzadeh, *Utilitas Mathematica*, **2011**, *84*, 297.
11. H. Wiener, *J. Am. Chem. Soc.*, **1947**, *69*, 17.
12. V. Sharma, R. Goswami, A.K. Madan, *J. Chem. Inf. Comput. Sci.,* **1997**, *37*, 273.
13. A.R. Ashrafi, M. Saheli, M. Ghorbani, *Journal of Computational and Applied Mathematics*, **2011**, *235*(16), 4561.
14. N. De, S.M.A. Nayeem, A. Pal, *Ann. Pure Appl. Math.,* **2014**, *7*(1), 59.
15. N. De, A. Pal, S.M.A. Nayeem, *Malaya J. Mat.*, **2015**, *3*(4), 523.
16. E. Estrada, L. Torres, L. Rodriguez, I. Gutman, *Indian Journal of Chemistry,* **1998**, *37*, 849.
17. D. Vukičević, B. Furtula, *Journal of Mathematical Chemistry*, **2009**, *46*, 1369.
18. M. Ghorbani, H. Hosseinzadeh, *Optoelectron. Adv. Mater. - Rapid Comm.*, **2010**, *4*, 1419.

19. A. Graovac, M. Ghorbani, M.A. Hosseinzadeh*, J. Math. Nanosci.*, **2011**, *1*, 33.
20. H. Shabani, A.R. Ashrafi, I. Gutman, *Studia UBB. Chemia*, **2010**, *4*, 107.
21. M. Higuchi, S. Shiki, K. Ariga, K. Yamamoto, *J. Am. Chem. Soc.*, **2001**, *123* (19), 4414.