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Eccentricity based topological indices of siloxane and POPAM dendrimers

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Abstract: A massive of early drug tests indicates that there is some strong inner connections among the bio-medical and pharmacology properties of nanostar dendrimers and their molecular structures. Topological descriptors are presented as fundamentally transforming a molecular graph into a number. There exist various categories of such descriptors particularly those descriptors that based on edge and vertex distances. Topological descriptors are exercised for designing biological, physico-chemical, toxicological, pharmacologic and other characteristics of chemical compounds. In this paper, we study infinite classes of siloxane and POPAM dendrimers and derive their Zagreb eccentricity indices, eccentric-connectivity and total-eccentricity indices.

Keywords: siloxane dendrimers; POPAM dendrimers; eccentricity based indices

1 Introduction

The mathematical sciences furnish the terminology for quantitative science, and this terminology is developing in many orientations as computational science in general continues its rapid development. A timely possibility now exists to grow and strengthen the useful impacts of chemistry by enhancing the relationship among the mathematical sciences and chemistry. Computational chemistry is a outgrowth of theoretical chemistry, the natural rule of which includes the construction and distribution of a penetrating conceptual infrastructure for the chemical sciences, at the atomic and molecular levels. The mathematical sciences have been crucial allies and have provided important tools for that rule.

Cheminformatics is a incorporation of mathematics, information science and chemistry. It interpretation quantitative structure-activity and quantitative structure-property correlation that are beneficial to save the biological activities and characteristics of various chemical compounds, see (Devillers and Balaban, 1999). In QSAR/QSPR investigation, physico-chemical characteristics and topological descriptors such as Wiener, Szeged, Randić, ABC and Zagreb indices are used to save the bioactivity of incompatible chemical compounds. If $\mathcal{G}$ presents the family of simple finite graphs then a topological descriptor $Top:\mathbb{G}_l \to \mathbb{R}$ is a function such that for any $\mathbb{G}_l, \mathbb{G}_m \in \mathcal{G}$, $Top(\mathbb{G}_l) = Top(\mathbb{G}_m)$ when $\mathbb{G}_l$ and $\mathbb{H}_m$ are both isomorphic. A graphical invariant is a quantity associated to a graph that is structural invariant.

Let $\mathbb{G}$ be a molecular simple and connected graph. The length of the smallest path along the vertices u and v is known as the distance among u and v. The degree of $w \in V(\mathbb{G})$, recognized as $d_{\mathbb{G}}(w)$, is the number of linked vertices to w in $\mathbb{G}$. The eccentricity of w is the greatest distance among w and any other vertex of $\mathbb{G}$.

The Wiener index, (Wiener, 1947), is investigated as half of the sum of the distances of all the pairs of vertices in $\mathbb{G}$. Also a distance based topological descriptor of $\mathbb{G}$ is the eccentric-connectivity $\xi(\mathbb{G})$ index (Sharma et al., 1997), interpreted as:

$$\xi(\mathbb{G}) = \sum_{w \in V(\mathbb{G})} d(w) \cdot \varepsilon(w)$$

and also the total eccentricity index of $\mathbb{G}$ presented by:

$$\varsigma(\mathbb{G}) = \sum_{u \in V(\mathbb{G})} \varepsilon(u)$$

For further aspects of these beneficial indices, please see: Ashrafi et al. (2009a), Ashrafi et al. (2009b), Ashrafi and Sadati (2009), Ashrafi and Saheli (2010), Akhter et al. (2018), Akhter and Imran (2016), Gao et al. (2019), Gupta et al. (2002), Iqbal et al. (2018), Iqbal et al. (2019), Yang et al. (2019), and Zhou and Du (2010).

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Zagreb eccentricity indices are investigated by (Ghorbani and Hosseinzadeh, 2012), and are expressed as:

$$M_1^*(\mathbb{G}) = \sum_{w \in V(\mathbb{G})} \left(\varepsilon(w)\right)^2$$

$$M_2^*(\mathbb{G}) = \sum_{wx \in E(\mathbb{G})} \varepsilon(w) \cdot \varepsilon(x)$$

For motivation and recent results on these topological indices related to the dendrimers, please see: Diudea et al. (2010), Malik and Farooq (2015a), Malik and Farooq (2015b), Zheng et al. (2019), and Iqbal et al. (2020).

In this paper, we consider POPAM and siloxane dendrimers, and work out their eccentricity topological indices. Also, we study the graphical comparison of eccentricity indices siloxane and POPAM dendrimers.

Dendrimers are hyper-branched macromolecule. They are being analyzed for their applications in nanotechnology, genetherapy and different areas. Each dendrimer consist of multi-functional core molecule with a dendritic wedge connected to each functional site. The core molecule without surrounding dendrons is commonly mentioned to as zero generations. Each successive iterative method along all branches forms every next generation, first generation and second generation until the terminating generation. Now a days, the topological investigation of this nanostructure has been a great interest of many researchers in chemical graph theory.

2 Some known results about siloxane and POPAM dendrimers

The ABC and GA indices of siloxane *SD*[r] and POPAM *PD*[r] dendrimers were studied in (Husin et al., 2015).

$$\mathrm{ABC}(SD[r]) = (3\sqrt{3}+3\sqrt{2})2^r - \sqrt{3} - 3\sqrt{2},$$
$$\mathrm{GA}(SD[r]) = (\frac{24}{5}+4\sqrt{2})2^r - \frac{8}{5} - 4\sqrt{2},$$
$$\mathrm{ABC}(PD[r]) = (16\times 2^r - \frac{11}{2})\sqrt{2}),$$
$$\mathrm{GA}(PD[r]) = (\frac{8}{3}\sqrt{2}+16+\frac{24}{5}\sqrt{6})2^r - 5 - \frac{12}{5}\sqrt{6}$$

The eccentricity based invariants of a hetrofunctional dendrimer were recently studied in (Farooq et al., 2015).

Now we consider the siloxane dendrimers (*SD*[r]) with trifunctional core unit with r growth stages. The graphs of siloxane dendrimers for r = 1 and r = 3 are presented

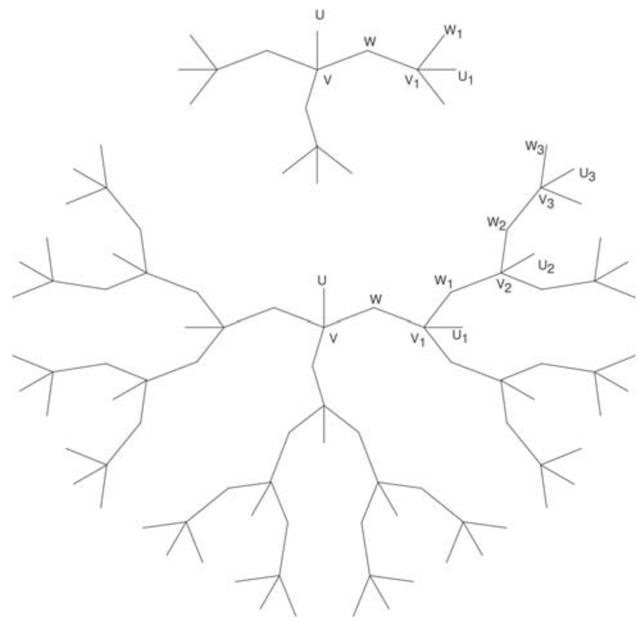

Figure 1: SD_1[r] for r = 1 and r = 3.

in Figure 1. The order and size of *SD*[r] are $3\times2^{r+2}$–7 and $3\times2^{r+2}$–8, respectively.

The POPAM dendrimer *PD*[r] with trifunctional core unit with r growth stages. The graphs of POPAM dendrimers for r = 1 and r = 3 are presented in Figure 2. The order and size of *PD*[r] are 2^{r+5}–10 and 2^{r+5}–11, respectively.

3 Main discussion and results

We start this section by computing the eccentric-connectivity index of SD_1[r] and *PD*[r] depicted in Figures 1 and 2, respectively.

Theorem 3.1

The eccentric-connectivity index of the siloxane nanostar dendrimer *SD*[r] is:

$$\xi(SD[r]) = (96r - 18)2^r - 32r + 30$$

Proof

As the structure of SD_1[r] is symmetric, so we take only one branch of *SD*[r] to obtain the result as located in Figure 1. We consider a representative from a *V*(*SD*[r]), which have same eccentricity and degree. These representatives are categorized by u, v, w, u_m, v_m, w_m for $1 \le m \le r$, and are presented in Table 1, along their rate of repetition.

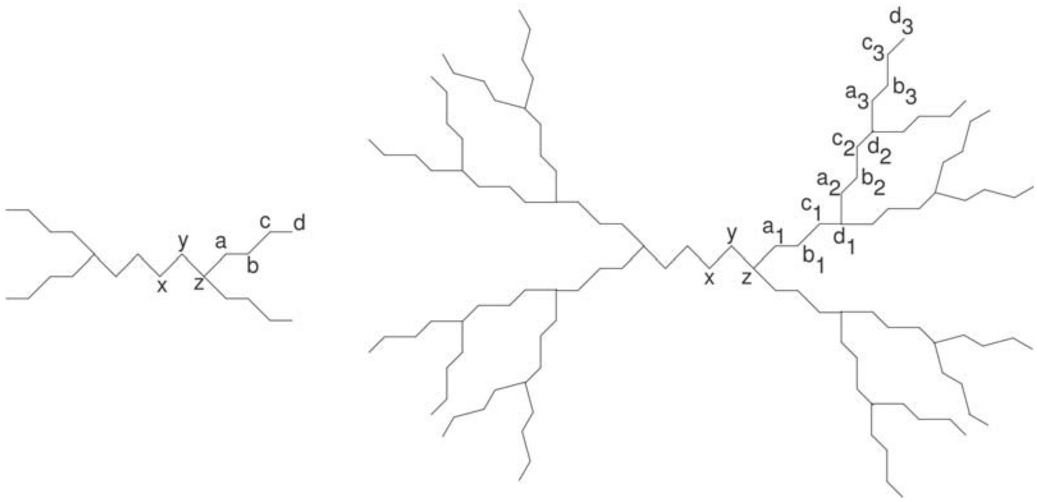

Figure 2: *PD*[r] with r = 1 and r = 3.

Table 1: The characterizations of elements of *V*(*SD*[r]).

Representatives	Degree	Eccentricity	Rate of repetition
U	1	2r+2	1
V	4	2r+1	1
W	2	2r+2	3
u_m	1	2r+2*m*+2	$3\times2^{m-1}$
v_m	4	2r+2*m*+1	$3\times2^{m-1}$
w_m	2(1 ≤ *m* ≤ r–1)	2r+2*m*+2	3×2^{m}
w_r	1	4r+2	3×2^{r}

Using Table 1, the eccentric-connectivity index of *SD*[r] for r ≥ 1, can be picked up as follows:

$$\xi(SD[\mathrm{r}])=\sum_{u\in V(SD_1[\ ])}(u)\cdot\varepsilon(u)$$
$$=1\times1\times(2r+2)+4\times1\times(2r+1)+2\times3\times(2r+2)$$
$$+\sum_{=1}^{r-1}\left(\begin{array}{l}1\times3\times2^{m-1}(2r+2m+2)+4\times3\times2^{m-1}(2r+2m+1)\\+2\times3\times2^{m}(2r+2m+2)\end{array}\right)$$
$$+1\times3\times2^{r-1}(4r+2)+4\times3\times2^{r-1}(4r+1)+1\times3\times2^{r}(4r+2)$$

After simplification, we get:

$$\xi(SD[\mathrm{r}])=(96r-18)2^{r}-32r+30$$

This completes the proof.

Theorem 2 provides eccentric-connectivity index of POPAM dendrimers *PD*[r].

Theorem 3.2

The eccentric-connectivity index of *PD*[r] is:

$$\xi(PD[\mathrm{r}])=(256r-32)2^{r}-88r+126$$

Table 2: The characterizations of elements of *V*(*PD*[r]).

Representatives	Vertex degree	Eccentricity	Frequency
x	2	4r+3	2
y	2	4r+4	2
z	3	4r+5	2
a_i	2	4r+4*m*+2	2^{m+1}
b_i	2	4r+4*m*+3	2^{m+1}
c_i	2	4r+4*m*+4	2^{m+1}
d_i	3(1 ≤ *m* ≤ r–1)	4r+4*m*+5	2^{m+1}
d_r	1	8r+5	2^{r+1}

Proof

Similarly here we take exactly one branch of *PD*[r] as marked in Figure 2. We pike up one representative from the *V*(*PD*[r] that have equal eccentricity and degree. These representatives are denoted by x, y, z, a_m, b_m, c_m, d_m for $1 \le m \le r$ are shown in Table 2 with their rate of repetition.

Using the statistics presented in Table 2, the eccentric-connectivity index of *PD*[r], for r ≥ 1, can be evaluated as:

$$\xi(PD[\mathrm{r}])=2\times2\times(4r+3)+2\times2\times(4r+4)+3\times2\times(4r+5)$$
$$+\sum_{m=1}^{r-1}\left[\begin{array}{l}2\times2^{m+1}\times(4r+4m+2)+2\times2^{m+1}\times(4r+4m+3)\\+2\times2^{m+1}\times(4r+4m+4)+3\times2^{m+1}\times(4r+4m+5)\end{array}\right]$$
$$+2\times2^{r+1}\times(8r+2)+2\times2^{r+1}\times(8r+3)+2\times2^{r+1}(8r+4)$$
$$+1\times2^{r+1}(8r+5)$$
$$\xi(SD[\mathrm{r}])=(96r-18)2^{r}-32r+30$$

which completes the proof.

Comparison of the eccentric-connectivity index ξ(*SD*[r]) and *PD*[r] is shown in Figure 3. It is easy to see

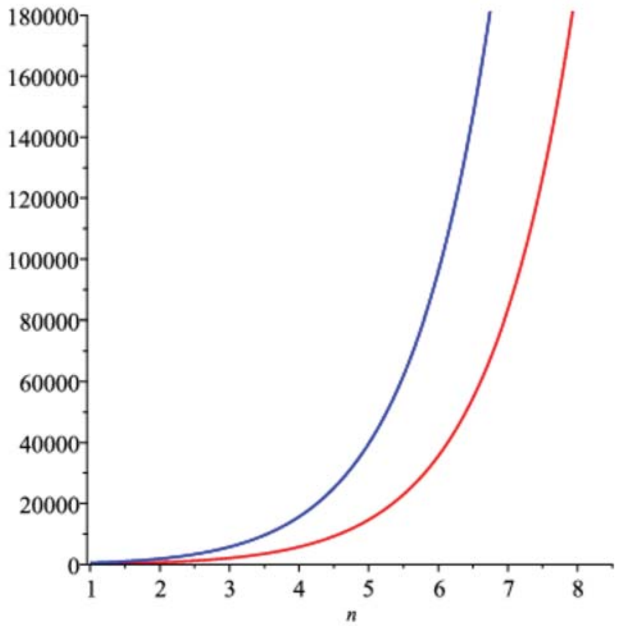

Figure 3: Comparison of the eccentric-connectivity index $\xi(SD[r])$ and $PD[r]$. The colors red and blue represents the eccentric-connectivity index $\xi(SD[r])$ and $PD[r]$, respectively. We can see that in the given domain the eccentric connectivity index of $PD[r]$ is more dominating.

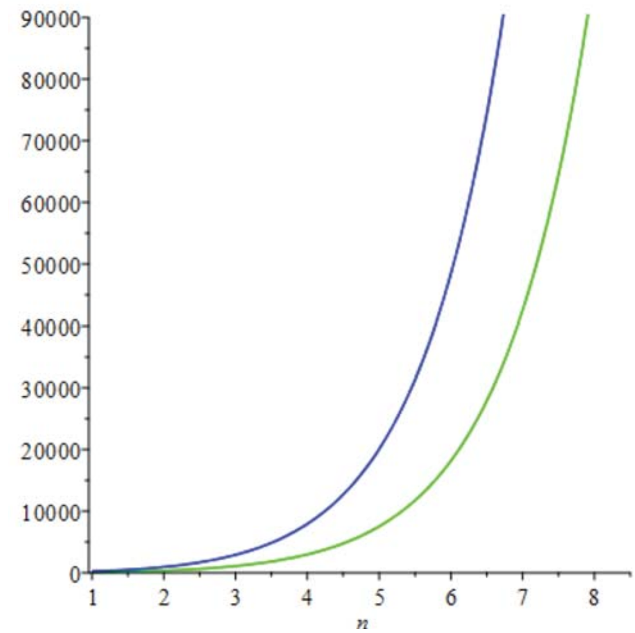

Figure 4: Comparison of the total-eccentricity index of $\varsigma(SD[r])$ and $PD[r]$. The colors green and blue represents the total-eccentricity index of $\varsigma(SD[r])$ and $PD[r]$, respectively. We can see that in the given domain the total-eccentricity index of $\xi(SD[r])$ is more dominating.

that in the given domain the eccentric connectivity index of $PD[r]$ is more dominating.

The upcoming two results can be easily established from Tables 1 and 2.

Corollary 3.1

The total-eccentricity index of siloxane nanostar dendrimers $SD[r]$ is:

$$\varsigma(SD[r]) = (48r-3)2^{r} - 14r + 12$$

Corollary 3.2

The total-eccentricity index of $PD[r]$ nanostar dendrimers is:

$$\varsigma(PD[r]) = (64r-4)2^{r+1} - 40r + 32$$

Figure 4 gives a comparison of the total-eccentricity index of $\varsigma(SD[r])$ and $PD[r]$. It is clear from Figure 4 that in the given domain the total-eccentricity index of $\xi(SD[r])$ is more dominating.

Now, we compute Zagreb eccentricity indices of the $SD[r]$ and $PD[r]$ nanostar dendrimers.

Theorem 3.3

The first Zagreb-eccentricity index of siloxane nanostar dendrimer $SD[r]$ is:

$$M_1^*(SD[r]) = (192r^2 - 24r + 99)2^{r} - 28r^2 + 48r - 82$$

Proof

From Table 1, we apply the values and evaluate the first Zagreb-eccentricity index of $SD[r]$ as follows:

$$\begin{aligned} M_1^*(SD[r]) &= \sum_{v \in V(SD_1[\ ])} [\varepsilon(v)]^2 \\ &= 1\times(2r+2)^2 + 1\times(2r+1)^2 + 3\times(2r+2)^2 \\ &\quad + \sum_{m=1}^{r} \begin{pmatrix} 3\times 2^{m-1}(2r+2m+2)^2 + 3\times 2^{m-1}(2r+2m+1)^2 \\ +3\times 2^{m}(2r+2m+2)^2 \end{pmatrix} \\ &= (192r^2 - 24r + 99)2^{r} - 28r^2 + 48r - 82 \end{aligned}$$

Theorem 3.4

The second Zagreb-eccentricity index of siloxane nanostar dendrimer $SD[r]$ is:

$$M_2^*(SD[r]) = (168r^2 - 54r + 87)2^{r} - 20r^2 + 66r - 70$$

Table 3: The edge distribution of *SD*[r] with reference to edges and their rate of occurrence. The eccentricities are picked up from Table 1.

Edges	Eccentricities	Rate of repetition
[u,v]	[2r+2,2r+1]	1
[v,w]	[2r+1,2r+2]	3
[w,v_1]	[2r+2,2r+3]	3
[v_m,u_m] ($1 \le m \le$ r)	[2r+2m+1,2r+2m+2]	$3\times2^{m-1}$
[v_m,w_m] ($1 \le m \le$ r)	[2r+2m+1,2r+2m+2]	3×2^{m}
[w_m,v_{m+1}] ($1 \le m \le$ r–1)	[2r+2m+2,2r+2m+3]	3×2^{m}

Proof

From Table 3, we apply the values and evaluate the second Zagreb-eccentricity index of *SD*[r] as follows:

$$\begin{aligned} M_2^*(SD[\mathrm{r}]) &= \sum_{uv\in\ (SD_1[\ ])} \varepsilon(\mathrm{u})\cdot\varepsilon(\mathrm{v}) \\ &= 1\times(2r+2)(2r+1)+3\times(2r+1)(2r+2) \\ &\quad +3\times(2r+2)(2r+3) \\ &\quad +\sum_{m=1}^{r}\begin{pmatrix} 3\times2^{m-1}(2r+2m+1)(2r+2m+2) \\ +3\times2^{m}(2r+2m+1)(2r+2m+2) \end{pmatrix} \\ &\quad +\sum_{m=1}^{r-1}\left(3\times2^{m}(2r+2m+2)(2r+2m+3)\right) \\ &= (168r^2-54r+87)2^r-20r^2+66r-70 \end{aligned}$$

This completes the result.

The comparison of first and second Zagreb-eccentricity index of siloxane nanostar dendrimer *SD*[r] is depicted in Figure 5. It is easy to verify that in the given domain the M_2^* (*SD*[r]) index of siloxane nanostar dendrimer *SD*[r] is more dominating.

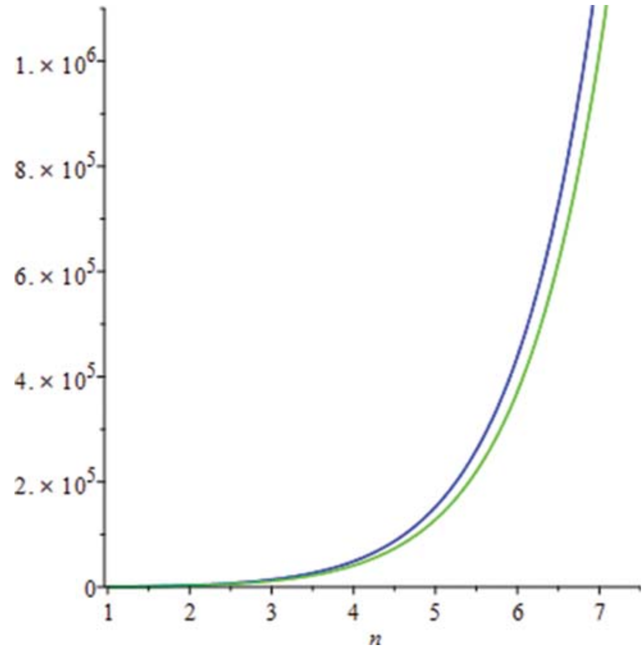

Figure 5: Comparison of first and second Zagreb-eccentricity index of siloxane nanostar dendrimer *SD*[r]. The colors blue and green represents the first and second Zagreb-eccentricity index of siloxane nanostar dendrimer *SD*[r], respectively. We can see that in the given domain the M_2^* (*SD*[r]) index of siloxane nanostar dendrimer *SD*[r] is more dominating.

Theorem 3.5

The first Zagreb-eccentricity index of PD_2 [r] is:

$$M_1^*(PD[\mathrm{r}]) = (512r^2-64r+268)2^{r+1}-160r^2+448r-148$$

Proof

We apply the values of Table 2 and evaluate the first Zagreb-eccentricity index of *PD*[r] as:

$$\begin{aligned} M_1^*(PD[\mathrm{r}]) &= 2\times(4r+3)^2+2\times(4r+4)^2+2\times(4r+5)^2 \\ &\quad +\sum_{m=1}^{r}\begin{bmatrix} 2^{m+1}\times(4r+4m+2)^2+2^{m+1}\times(4r+4m+3)^2 \\ +2^{m+1}\times(4r+4m+4)^2+2^{m+1}\times(4r+4m+5)^2 \end{bmatrix} \\ &= (512r^2-64r+268)2^{r+1}-160r^2+256r-436 \end{aligned}$$

which completes the result.

Theorem 3.6

The second Zagreb-eccentricity index of *PD*[r] is:

$$M_2^*(PD[\mathrm{r}]) = (192r^2-24r+98)2^{2+r}+(256r^2-160r+152)2^r-176r^2 +280r-471$$

Proof

We compute the second Zagreb-eccentricity index of *PD*[r] by use of Table 4 as:

$$\begin{aligned} M_2^*(PD[\mathrm{r}]) &= 1\times(4r+3)(4r+3)+2\times(4r+3)(4r+4) \\ &\quad +2\times(4r+4)(4r+5)+4\times(4r+5)(4r+6) \\ &\quad +\sum_{m=1}^{r}\begin{bmatrix} 2^{m+1}(4r+4m+2)(4r+4m+3) \\ +2^{m+1}(4r+4+3)(4r+4+4) \\ +2^{m+1}(4r+4m+4)(4r+4m+5) \end{bmatrix} \\ &\quad +\sum_{m=1}^{r-1}2^{m+2}(4r+4m+5)(4r+4m+6) \\ &= (192r^2-24r+98)2^{2+r}+(256r^2-160r+152)2^r \\ &\quad -176r^2+280r-471 \end{aligned}$$

This gives the required result.

Table 4: The edge distribution of *PD*[r] with reference to edges and their rate of occurrence. The eccentricities are picked up from Table 2.

Edges	Eccentricities	Rate of repetition
[x,x]	[4r+3,4r+3]	1
[x,y]	[4r+3,4r+4]	2
[y,z]	[4r+4,4r+5]	2
$[z,a_1]$	[4r+5,4r+6]	4
$[a_m,b_m]$ $(1 \le m \le r)$	$[4r+4m+2,4r+4m+3]$	2^{m+1}
$[b_m,c_m]$ $(1 \le m \le r)$	$[4r+4m+3,4r+4m+4]$	2^{m+1}
$[c_m,d_m]$ $(1 \le m \le r)$	$[4r+4m+4,4r+4m+5]$	2^{m+1}
$[d_m,a_{m+1}]$ $(1 \le m \le r-1)$	$[4r+4m+5,4r+4m+6]$	2^{m+2}

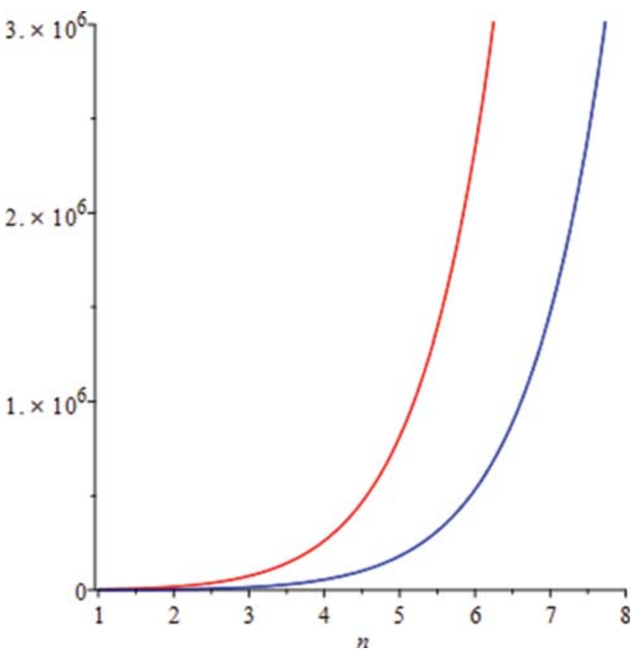

Figure 6: Comparison of first Zagreb-eccentricity index of *PD*[r] and second Zagreb eccentricity index of *PD*[r]. The colors red and blue represents the first and second Zagreb-eccentricity indices of *PD*[r], respectively. We can see that in the given domain M_1^* (*PD*[r]) is more dominating.

In Figure 6, comparison of first Zagreb-eccentricity index of PD[r] and second Zagreb eccentricity index of *PD*[r] which shows that in the given domain M_1^* (*PD*[r]) is more dominating.

All above results are concluded in the following Table 5.

Table 5: Concluded results.

Indices	Results
$\xi(SD[r])$	$(96r-18)2^r-32r+30$
$\xi(PD[r])$	$(256r-32)2^r-88r+126$
$\varsigma(SD[r])$	$(48r-3)2^r-14r+12$
$\varsigma(PD[r])$	$(64r-4)2^{r+1}-40r+32$
$M_1^*(SD[r])$	$(192r^2-24r+99)2^r-28r^2+48r-82$
$M_2^*(SD[r])$	$(168r^2-54r+87)2^r-20r^2+66r-70$
$M_1^*(PD[r])$	$(512r^2-64r+268)2^{r+1}-160r^2+448r-148$
$M_2^*(PD[r])$	$(192r^2-24r+98)2^{2+r}+(256r^2-160r+152)2^r-176r^2+280r-471$

4 Conclusion

In this paper, we study siloxane and POPAM nanostar dendrimers and figure out their eccentric-connectivity, total-eccentricity, Zagreb-eccentricity indices and certain new formulas are obtained. Moreover we represents the comparison of the eccentric-connectivity index ξ(*SD*[r]) and the eccentric-connectivity index of *PD*[r] graphically. Also, graphically we represents the comparison of the total-eccentricity index ξ(*SD*[r]) and the total-eccentricity index of *PD*[r]. Finally we represents the comparison of Zagreb-eccentricity indices of siloxane nanostar dendrimer *SD*[r], and also presents the comparison of Zagreb-eccentricity indices of *PD*[r]. Next, we are focused to figure out certain new architectures and determine their topological descriptors which will be useful to recognize their topologies.

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