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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 an 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 an 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 $G$ presents the family of simple finite graphs then a topological descriptor $\text{Top}:G\rightarrow \mathbb{R}$ is a function such that for any $G_1, G_2 \in G$, $\text{Top}(G_1) = \text{Top}(G_2)$ when $G_1$ and $G_2$ are both isomorphic.

A graphical invariant is a quantity associated to a graph that is structural invariant.

Let $G$ 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 $w \in V(G)$, recognized as $d_G(w)$, is the number of linked vertices to $w$ in $G$. The eccentricity of $w$ is the greatest distance among $w$ and any other vertex of $G$.

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

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

and also the total eccentricity index of $G$ presented by:

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

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

\[ M_1'(G) = \sum_{w \in V(G)} (\varepsilon(w))^2 \]

\[ M_2'(G) = \sum_{w \in V(G)} \varepsilon(w) \varepsilon(x) \]

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 nano-structure 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).

\[
ABC(SD[r]) = (3\sqrt{3} + 3\sqrt{2})2^r - \sqrt{3} - 3\sqrt{2},
\]

\[
GA(SD[r]) = (24 + 4\sqrt{2})2^r - \frac{8}{5} - 4\sqrt{2},
\]

\[
ABC(PD[r]) = (16\times 2^r - \frac{11}{2})\sqrt{2},
\]

\[
GA(PD[r]) = (\frac{8}{3}\sqrt{2} + 16 + \frac{24}{5})2^r - 5\sqrt{6} - \frac{12}{5}\sqrt{6}.
\]

The eccentricity based invariants of a heterofunctional 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 in Figure 1. The order and size of SD[r] are 3×2[r^2−7] and 3×2[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^2−10] and 2[r^2−11], respectively.

3 Main discussion and results

We start this section by computing the eccentric-connectivity index of SD[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[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, v, w for 1 ≤ m ≤ r, and are presented in Table 1, along their rate of repetition.
Using Table 1, the eccentric-connectivity index of $SD[r]$ for $r \geq 1$, can be picked up as follows:

$$
\xi(SD[r]) = \sum_{u \in V(SD[r])} (u \cdot \varepsilon(u)) - 1 \times 1 \times (2r+2) + 4 \times 1 \times (2r+1) + 2 \times 3 \times (2r+2)
+ \sum_{m=1}^{r-1} \left[ 1 \times 3 \times 2^{m-1} \times (2r+2m+2) + 4 \times 3 \times 2^{m-1} \times (2r+2m+1) \right]
+ 1 \times 3 \times 2^{m-1} \times (4r+2) + 4 \times 3 \times 2^{m-1} \times (4r+1) + 1 \times 3 \times 2^{m-1} \times (4r+2)
$$

After simplification, we get:

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

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:

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

which completes the proof.

Similarly, here we take exactly one branch of $PD[r]$ as marked in Figure 2. We take up one representative from the $V(PD[r])$ that have equal eccentricity and degree. These representatives are denoted by $x$, $y$, $z$, $a_i$, $b_i$, $c_i$, $d_i$ for $1 \leq m \leq r$ 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 $r \geq 1$, can be evaluated as:

$$
\xi(PD[r]) = 2 \times 2 \times (4r+3) + 2 \times 2 \times (4r+4) + 3 \times 2 \times (4r+5)
+ \sum_{m=1}^{r-1} \left[ 2 \times 2^{m-1} \times (4r+4m+2) + 2 \times 2^{m-1} \times (4r+4m+3) \right]
+ 2 \times 2^{r-1} \times (8r+2) + 2 \times 2^{r-1} \times (8r+3) + 2 \times 2^{r-1} \times (8r+4)
+ 1 \times 2^{r-1} \times (8r+5)
$$

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

which completes the proof.
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:

\[
\zeta(SD[r]) = (48r - 3)2^r - 14r + 12
\]

### Corollary 3.2

The total-eccentricity index of \( PD[r] \) nanostar dendrimers is:

\[
\zeta(PD[r]) = (64r - 4)2^r - 40r + 32
\]

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

\[
M_1^*(SD[r]) = \sum_{v \in V(SD[r])} |e(v)|^2
\]

\[
= 1 \times (2r+2)^2 + 1 \times (2r+1)^2 + 3 \times (2r+2)^2
\]

\[
+ \sum_{m=1}^{\infty} \left( 3 \times 2^{m-2} (2r+2m+2)^2 + 3 \times 2^{m-1} (2r+2m+1)^2 \right)
\]

\[
= (192r^2 - 24r + 99)2^r - 28r^2 + 48r - 82
\]

### 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 |
| $[w,v]$ | $[2r+2,2r+3]$ | 3 |
| $[v_m,u_n]$ ($1 \leq m \leq r$) | $[2r+2m+1,2r+2m+2]$ | $3 \times 2^{m-1}$ |
| $[v_m,w_n]$ ($1 \leq m \leq r$) | $[2r+2m+1,2r+2m+2]$ | $3 \times 2^m$ |
| $[w_m,v_n]$ ($1 \leq m \leq r-1$) | $[2r+2m+2,2r+2m+3]$ | $3 \times 2^m$ |

Proof

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

$$M_2^*(SD[r]) = \sum_{uv \in SD[r]} c(u) \cdot c(v)$$

$$= 1 \times (2r+2)(2r+1) + 3 \times (2r+1)(2r+2) + 3 \times \sum_{m=1}^{r-1} \left( 3 \times 2^{m-1} (2r+2m+1)(2r+2m+2) / 2 + 3 \times 2^m (2r+2m+1)(2r+2m+2) / 2 \right)$$

$$+ \sum_{m=1}^{r-1} \left( 3 \times 2^{m-1} (2r+2m+2)(2r+2m+3) / 2 \right)$$

$$= (168r^3 - 54r + 87)2^r - 20r^2 + 66r - 70$$

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.

Theorem 3.6

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

$$M_2^*(PD[r]) = (192r^2 - 24r + 98)2^{-2r} + (256r^2 - 160r + 152)2^{1-r} - 176r^2 + 280r - 471$$

Proof

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

$$M_2^*(PD[r]) = 1 \times (4r+3)(4r+3) + 2 \times (4r+4)(4r+5) + 4 \times (4r+5)(4r+6)$$

$$+ \sum_{m=1}^{r-1} \left[ 2^{m-1} (4r+4m+2)(4r+4m+3) + 2^{m-1} (4r+4m+4)(4r+4m+5) \right]$$

$$+ \sum_{m=2}^{r-1} (4r+4m+5)(4r+4m+6)$$

$$= (192r^2 - 24r + 98)2^{-2r} + (256r^2 - 160r + 152)2^{1-r} - 176r^2 + 280r - 471$$

This gives the required result.
respectively. We can see that in the given domain $M_1$ represents the first and second Zagreb-eccentricity indices of total-eccentricity, Zagreb-eccentricity indices and certain dendrimers and figure out their eccentric-connectivity, in this paper, we study siloxane and POPAM nanostar and POPAM 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 $\xi(\text{SD}[r])$ and the eccentric-connectivity index of $PD[r]$ graphically. Also, graphically we represents the comparison of the total-eccentricity index $\xi(\text{SD}[r])$ 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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### References

Ashrafi A.R., Ghorbani M., Jalali M., Eccentric connectivity polynomial of an infinite family of Fullerenes. Optoelectron. Adv. Mater. Rapid Comm., 2009a, 3, 823-826.

Ashrafi A.R., Nikzad P., Austin K., Connectivity index of the family of dendrimers nanostars. Digest J. Nanomater. Biostruct., 2009b, 4, 269-273.

Ashrafi A.R., Sadati M., Eccentric connectivity polynomial of an infinite family of fullerenes. Optoelectron. Adv. Mater. Rapid Comm., 2009, 3(8), 821-822.

Ashrafi A.R., Saheli M., The eccentric connectivity index of a new class of nanostar dendrimers. Optoelectron. Adv. Mater. Rapid Comm., 2010, 4(6), 898-899.

Akhter S., Imran M., Gao W., Frahani M.R., On topological indices of honeycomb networks and Graphene networks. Hacetettepe J. Math. Stat., 2018, 47(1), 1-17.

Akhter S., Imran M., On degree-based topological descriptors of strong product graphs. Can. J. Chem., 2016, 94(6), 559-565.

In this paper, we study siloxane and POPAM nanostar dendrimers and figure out their eccentric-connectivity, total-eccentricity, Zagreb-eccentricity indices and certain

### 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]         | [4r + 5, 4r + 6]     | 4                  |
| [a,b] (1 ≤ m ≤ r) | [4r + 4m + 2, 4r + 4m + 3] | 2^(m+1) |
| [b,c] (1 ≤ m ≤ r) | [4r + 4m + 3, 4r + 4m + 4] | 2^(m+1) |
| [c,d] (1 ≤ m ≤ r) | [4r + 4m + 4, 4r + 4m + 5] | 2^(m+1) |
| [d,e] (1 ≤ m ≤ r) | [4r + 4m + 5, 4r + 4m + 6] | 2^(m+2) |

In 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 $M'_2(PD[r])$ 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 $M'_2(PD[r])$ is more dominating.

All above results are concluded in the following Table 5.

### Table 5: Concluded results.

| Indices          | Results                                                               |
|------------------|----------------------------------------------------------------------|
| $\xi(\text{SD}[r])$ | $(96r−18)r^2−32r+30$                                                  |
| $\xi(\text{PD}[r])$ | $(256r−32)r^2−88r+126$                                              |
| $\zeta(\text{SD}[r])$ | $(48r−3)r^2−14r+12$                                                  |
| $\zeta(\text{PD}[r])$ | $(64r−4)r^2−40r+32$                                                  |
| $M'_1(\text{SD}[r])$ | $(192r^2−24r+99)r^2−28r^2+48r−82$                                   |
| $M'_1(\text{SD}[r])$ | $(168r^2−54r+87)r^2−20r^2+66r−70$                                   |
| $M'_1(\text{PD}[r])$ | $(512r^2−64r+268)r^2−160r^2+448r−148$                                |
| $M'_1(\text{PD}[r])$ | $(192r^2−24r+98)r^2−28r^2+(256r^2−160r+152)r^2−176r^2+280r−471$   |
Diudea M.V., Vizitiu A.E., Mirzargar M., Ashrafi A.R., Sadhana polynomial in nano-dendrimers. Carpathian J. Math., 2010, 26, 59-65.

Devillers J., Balaban A.T., Topological Indices and Related Descriptors in QSAR and QSPPR. Gordon & Breach, Amsterdam, 1999.

Farooq R., Nazir N., Malik M.A., Arfan M., Eccentricity based topological indices of a heterofunctional dendrimer. J. Optoelectron. Adv. Mater., 2015, 17, 1799-1807.

Gao W., Iqbal Z., Ishaq M., Aslam A., Sarfraz R., Topological aspects of dendrimers via distance-based descriptors. IEEE Access, 2019, 7, 35619-35630.

Ghorbani M., Hosseinzadeh M.A., A new version of Zagreb indices, Filomat, 2012, 26(1), 93-100.

Gupta S., Singh M., Madan A.K., Application of graph theory: Relationship of eccentric connectivity index and Wiener’s index with anti-inflammatory activity. J. Math. Anal. Appl., 2002, 266, 259-268.

Husin N.M., Hasni R., Arif N.E., Atom bond connectivity and geometric arithmetic indices of POPAM and siloxane dendrimers. J. Comput. Theor. Nanosci., 2015, 12, 1-4.

Iqbal Z., Aslam A., Ishaq M., Gao W., The edge version of degree-based topological indices of dendrimers. J. Cluster Sci., 2020, 31, 445-452.

Iqbal Z., Ishaq M., Aamir M., On eccentricity-based topological descriptors of dendrimers. Iran. J. Sci. Technol. Trans. A-Sci., 2019, 43, 1523-1533.

Iqbal Z., Ishaq M., Aslam A., Gao W., On eccentricity-based topological descriptors of water-soluble dendrimers. Z. Naturforsch. C-Biosci., 2018, 74(1), 25-33.

Malik M.A., Farooq R., Computational results on the energy and Estrada index of $\text{TUC}_4(C(R)[m,n])$ nanotubes. Optoelectron. Adv. Mater. Rapid Comm., 2015a, 9(1), 311-313.

Malik M.A., Farooq R., Some conjectures on energy and Estrada index of $\text{CN}_4[n]$ nanocones. Optoelectron. Adv. Mater. Rapid Comm., 2015b, 9(5), 415-418.

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

Wiener H., Structural determination of the paraffin boiling points. J. Am. Chem. Soc., 1947, 69, 17-20.

Yang H., Imran M., Akhter S., Iqbal Z., Siddiqui M.K., On distance-based topological descriptors of subdivision vertex-edge join of three graphs. IEEE Access, 2019, 7, 143381-143391.

Zhou B., Du Z., On eccentric connectivity index. MATCH Commun. Math. Comput. Chem., 2010, 63, 181-198.

Zheng J., Iqbal Z., Fahad A., Zafar A., Aslam A., Qureshi M.I, et al., Some eccentricity-based topological indices and polynomials of poly(ETHyleneAmidoAmine) (PETAA) dendrimers. Processes, 2019, 7, 433.