Research Article

Computing Zagreb and Randić Indices of PEG-Cored Dendrimers Used for Drug and Gene Delivery

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Zagreb and Randić indices are the most commonly used degree-based topological indices in the study of drug design and development. In molecular topology, M -polynomials are also used to calculate the degree-based topological indices of chemical structures. In this paper, we derive the M -polynomials for the PEG-cored PAMAM, carbosilane, and poly (lysine) dendrimers and calculate their first, second, and second modified Zagreb indices and the Randić index.

1. Introduction

A topological index is a numerical quantity, which is derived mathematically in a direct and unambiguous manner from the structural graph of a molecule. They are calculated from the heavy atom graphical depiction of the molecule. The most commonly used topological indices in the field of drug design and development are the Wiener index, Kosyano index or Z index, Zagreb index, Randić index, and Balaban J index. Among these indices, the Wiener index, Kosyano index or Z index, and Balaban J indices are nondegree -based topological indices, while Zagreb and Randić indices are the degree-based topological indices. The degree-based topological indices are the most studied type of topological indices, which play an important role in the field of molecular graph theory or molecular topology. Topological indices are mostly used in the drug design and development process, and some of their roles are reported by researchers [1–5]. Recent studies on Zagreb and Randić indices are reported by various scientists [6–9]. Nowadays, many researchers are focused on dendrimers to study their various topological indices [10–12].

Dendrimers are manmade, nanoscale compounds with unique properties that make them useful in many

applications, especially in the field of medical applications. These dendrimers are monodisperse molecule with a regular and highly branched three-dimensional architecture. The globular structure and excellent flexibility of dendrimers make them as a drug and gene delivery system [13–15].

In this work, we considered three types of PEG-cored dendrimers such as PEG-cored PAMAM, PEG-cored carbosilane, and PEG-cored triazine, and these dendrimers are used as promising candidates for drug and gene delivery with high drug encapsulation, sustained release behaviour, and excellent gene transfection efficiency. In this paper, we computed Zagreb index and Randić index for the above-mentioned PEG-cored dendrimers, and these results could be used in determining properties of these compounds [16].

A molecular graph in the molecular graph theory or molecular topology is a simple graph which has neither loops nor multiple edges. In the molecular graph theory, the atoms and the chemical bonds between atoms are represented by vertices and edges, respectively. A graph $G = G(V, E)$ consists of a nonempty set of vertices $V = V(G)$ and the set of connected edges (if there exists a connection between any pair of vertices) $E = E(G)$. In a connected graph, the degree of v is denoted by $d_v(G)$ or d_v and is defined to be the number of vertices which are

connected to that vertex by the edges. The concept of degree is closely related to the concept of valence bond in chemistry. The distance between two vertices u and v is denoted by $d(u, v)$ or $d_G(u, v)$ and is defined to be the length of shortest path between these vertices.

The Wiener index is the first and the most studied distance-based topological index in molecular topology. This was introduced by a chemist, Wiener [17] in 1947, to demonstrate the correlations between physicochemical properties of organic compounds and the topological structure of their molecular graphs. The Wiener index is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v). \quad (1)$$

This is calculated as the sum of distances between all the carbon atoms in the molecules, in terms of carbon-carbon bonds. Wiener named this index as the path number. The degree-based topological indices are the second type of topological indices, which are the most studied type of topological indices in molecular topology. One of the oldest degree-based topological indices is the well-known Zagreb index, which was introduced by Gutman and Trinajstić [18] in 1972 during the analysis of the structure-dependency of total π -electron energy. The name Zagreb is the place where both of them worked in an institute as members of the theoretical chemistry group. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ s are defined as

$$\begin{aligned} M_1(G) &= \sum_{v \in V(G)} (d_v)^2 = \sum_{uv \in E(G)} (d_u + d_v), \\ M_2(G) &= \sum_{uv \in E(G)} d_u d_v. \end{aligned} \quad (2)$$

The second modified Zagreb index [19] is defined as

$${}^m M_2 M_2(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v}. \quad (3)$$

Another oldest degree-based topological index called as the Randić index was introduced by Randić [20] in 1974 and defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}. \quad (4)$$

Randić named this index as the branching index, and soon, it was renamed as connectivity index. The Randić index is the most studied and most often applied degree-based topological index in the field of drug design. This index was globalized and called as the generalized Randić index [21]. The generalized Randić index is defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha, \quad (5)$$

where α is an arbitrary real number. The Randić index could be obtained from this formula by substituting $\alpha = -1/2$.

2. Materials and Methods

Many graph polynomials play a prominent role to study the structural properties of the molecules. Among them, the Hosoya polynomial (also known as the Wiener polynomial) plays a vital role to determine the distance-based topological indices. Among the graph polynomials, the M -polynomial, which was introduced in 2015 by Deutsch and Klavzar [22], plays another important role to determine many degree-based topological indices.

For a graph $G = G(V, E)$, the M -polynomial is defined as

$$M(G; x, y) = \sum_{i \leq j} m_{ij}(G) x^i y^j, \quad (6)$$

where $m_{ij}(G)$, $i, j \geq 1$ is the number of edges $e = uv$ of G such that $\{d_u, d_v\} = \{i, j\}$, and $u, v \in V(G)$. The derived formulas to compute Zagreb and Randić indices from the M -polynomial are given in Table 1.

Here, $D_x = x \partial f(x, y) / \partial x$, $D_y = y \partial f(x, y) / \partial y$, $S_x = \int_0^x f(t, y) / t dt$, and $S_y = \int_0^y f(x, t) / t dt$.

In this paper, we considered the three dendrimers, PEG-cored PAMAM dendrimer (Figure 1), PEG-cored carbosilane dendrimer (Figure 2), and PEG-cored triazine dendrimer (Figure 3), which are used for drug and gene delivery. We first calculate the M -polynomial and then find the first, second, and the second modified Zagreb indices and the Randić index for each of the dendrimer using the formulas in Table 1.

3. Results

Theorem 1. Let G be the PEG-cored PAMAM dendrimer. Then, the M -polynomial for G is given as

$$\begin{aligned} M(C_{60}, x, y) &= 2 \times 4^n x y^2 + 4(4^n - 1) x y^3 \\ &\quad + (12 \times 4^n + 3n - 13) x^2 y^2 \\ &\quad + (12 \times 4^n - 6) x^2 y^3. \end{aligned} \quad (7)$$

Proof. There are four types of edge partitions based on degrees of end vertices of each edge for the PEG-cored PAMAM dendrimer G given in Figure 1. The first edge partitions E_{12} contains 2×4^n edges, where $d_u = 1$ and $d_v = 2$. The second edge partition E_{13} contains $4(4^n - 1)$ edges, where $d_u = 1$ and $d_v = 3$. The third edge partition E_{22} contains $(12 \times 4^n + 3n - 13)$ edges, where $d_u = d_v = 2$. The fourth edge partition E_{23} contains $(12 \times 4^n - 6)$ edges, where $d_u = 2$ and $d_v = 3$.

Therefore, the M -polynomial of G is

$$\begin{aligned} M(G, x, y) &= \sum_{i \leq j} m_{ij} x^i y^j = 2 \times 4^n x y^2 + 4(4^n - 1) x y^3 \\ &\quad + (12 \times 4^n + 3n - 13) x^2 y^2 \\ &\quad + (12 \times 4^n - 6) x^2 y^3. \end{aligned} \quad (8)$$

□

TABLE 1: The derived formulas to compute some degree-based topological indices from M -polynomial [18].

Topological index	$f(x, y)$	Derivation from $M(G; x, y)$
First Zagreb— $M_1(G)$	$x + y$	$(D_x + D_y)(M(G; x, y))_{x=y=1}$
Second Zagreb— $M_2(G)$	xy	$(D_x D_y)(M(G; x, y))_{x=y=1}$
Second modified Zagreb— ${}^m M_2(G)$	$1/xy$	$(S_x S_y)(M(G; x, y))_{x=y=1}$
General Randić— $R_\alpha(G)$, $\alpha \in \mathbb{N}$	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha)(M(G; x, y))_{x=y=1}$

FIGURE 1: The structure of PEG-cored PAMAM dendrimer [16].

Proposition 1. The first Zagreb index $M_1(G)$, second Zagreb index $M_2(G)$, second modified Zagreb index ${}^m M_2(G)$, and general Randić index $R_\alpha(G)$, where $\alpha \in \mathbb{N}$, for the PEG-cored PAMAM dendrimer G are given as

$$(1) M_1(G) = 130 \times 4^n + 12n - 98$$

$$(2) M_2(G) = 136 \times 4^n + 12n - 100$$

$$(3) {}^m M_2(G) = (22/3) \times 4^n + (3/4)n - (67/4)$$

$$(4) R(G) = (\sqrt{2} + (4/\sqrt{3}) + (12/\sqrt{6}) + 6) \times 4^n + (3/2)n - ((13/2) + (4/\sqrt{3}) + (6/\sqrt{6}))$$

Proof. Let $f(x, y)$ be the M -polynomial of G . Then,

FIGURE 2: PEG-cored carbosilane dendrimer [16].

FIGURE 3: PEG-cored triazine dendrimer [16].

$$\begin{aligned}
D_x(f(x, y)) &= 2 \times 4^n xy^2 + 4(4^n - 1)xy^3 + 2(12 \times 4^n + 3n - 13)x^2y^2 + 2(12 \times 4^n - 6)x^2y^3, \\
D_y(f(x, y)) &= 4 \times 4^n xy^2 + 12(4^n - 1)xy^3 + 2(12 \times 4^n + 3n - 13)x^2y^2 + 3(12 \times 4^n - 6)x^2y^3, \\
D_x D_y(f(x, y)) &= 4 \times 4^n xy^2 + 12(4^n - 1)xy^3 + 4(12 \times 4^n + 3n - 13)x^2y^2 + 6(12 \times 4^n - 6)x^2y^3, \\
S_y(f(x, y)) &= 4^n xy^2 + \frac{4}{3}(4^n - 1)xy^3 + \frac{1}{2}(12 \times 4^n + 3n - 13)x^2y^2 + \frac{1}{3}(12 \times 4^n - 6)x^2y^3, \\
S_x S_y(f(x, y)) &= 4^n xy^2 + \frac{4}{3}(4^n - 1)xy^3 + \frac{1}{4}(12 \times 4^n + 3n - 13)x^2y^2 + \frac{1}{6}(12 \times 4^n - 6)x^2y^3, \\
D_y^\alpha(f(x, y)) &= 2^{\alpha+1} \times 4^n xy^2 + 4 \times 3^\alpha(4^n - 1)xy^3 + 2^\alpha \times (12 \times 4^n + 3n - 13)x^2y^2 + 3^\alpha \times (12 \times 4^n - 6)x^2y^3, \\
D_x^\alpha D_y^\alpha(f(x, y)) &= 2^{\alpha+1} \times 4^n xy^2 + 4 \times 3^\alpha(4^n - 1)xy^3 + 4^\alpha \times (12 \times 4^n + 3n - 13)x^2y^2 + 6^\alpha \times (12 \times 4^n - 6)x^2y^3.
\end{aligned} \tag{9}$$

Using the derived formulas of M -polynomial given in Table 1, we find

- (1) $M_1(G) = (D_x + D_y)(f(x, y))|_{x=y=1} = 130 \times 4^n + 12n - 98$
- (2) $M_2(G) = D_x D_y(f(x, y))|_{x=y=1} = 136 \times 4^n + 12n - 100$
- (3) ${}^m M_2(G) = S_x S_y(f(x, y))|_{x=y=1} = (22/3) \times 4^n + (3/4)n - (67/4)$
- (4) $R(G) = D_x^\alpha D_y^\alpha(f(x, y))|_{x=y=1, \alpha=-1/2} = (\sqrt{2} + (4/\sqrt{3}) + (12/\sqrt{6}) + 6) \times 4^n + (3/2)n - ((13/2) + (4/\sqrt{3}) + (6/\sqrt{6}))$ $\square$

Theorem 2. Let G be the PEG-cored carbosilane dendrimer. Then, the M -polynomial for G is given as

$$M(C_{60}, x, y) = 6 \times 3^n xy^2 + (11 \times 3^n + 3n - 6)x^2y^2 + (12 \times 3^n - 4)x^2y^4. \tag{10}$$

Proof. There are three types of edge partitions based on degrees of end vertices of each edge for the PEG-cored carbosilane dendrimer G given in Figure 2. The first edge partitions E_{12} contains 6×3^n edges, where $d_u = 1$ and $d_v = 2$.

The second edge partition E_{22} contains $(11 \times 3^n + 3n - 6)$ edges, where $d_u = d_v = 2$. The third edge partition E_{24} contains $(12 \times 3^n - 4)$ edges, where $d_u = 2$ and $d_v = 4$.

Therefore, the M -polynomial of G is

$$\begin{aligned}
M(G, x, y) &= \sum_{i \leq j} m_{ij} x^i y^j = 6 \times 3^n xy^2 \\
&\quad + (11 \times 3^n + 3n - 6)x^2y^2 \\
&\quad + (12 \times 3^n - 4)x^2y^4.
\end{aligned} \tag{11}$$

$\square$

Proposition 2. The first Zagreb index $M_1(G)$, second Zagreb index $M_2(G)$, second modified Zagreb index ${}^m M_2(G)$, and general Randić index $R_\alpha(G)$, where $\alpha \in \mathbb{N}$, for the PEG-cored carbosilane dendrimer G are given as

- (1) $M_1(G) = 134 \times 3^n + 12n - 48$
- (2) $M_2(G) = 152 \times 3^n + 12n - 56$
- (3) ${}^m M_2(G) = (29/4) \times 3^n + (3/4)n - 2$
- (4) $R(G) = (6\sqrt{2} + (11/2)) \times 3^n + (3/2)n - (3 + \sqrt{2})$

Proof. Let $f(x, y)$ be the M -polynomial of G . Then,

$$\begin{aligned}
D_x(f(x, y)) &= 6 \times 3^n xy^2 + 2(11 \times 3^n + 3n - 6)x^2y^2 + 2(12 \times 3^n - 4)x^2y^4, \\
D_y(f(x, y)) &= 12 \times 3^n xy^2 + 2(11 \times 3^n + 3n - 6)x^2y^2 + 4(12 \times 3^n - 4)x^2y^4, \\
D_x D_y(f(x, y)) &= 12 \times 3^n xy^2 + 4(11 \times 3^n + 3n - 6)x^2y^2 + 8(12 \times 3^n - 4)x^2y^4, \\
S_y(f(x, y)) &= 3 \times 3^n xy^2 + \frac{(11 \times 3^n + 3n - 6)}{2}x^2y^2 + (3 \times 3^n - 1)x^2y^4, \\
S_x S_y(f(x, y)) &= 3 \times 3^n xy^2 + \frac{(11 \times 3^n + 3n - 6)}{4}x^2y^2 + \frac{(3 \times 3^n - 1)}{2}x^2y^4, \\
D_y^\alpha(f(x, y)) &= 6 \times 2^\alpha \times 3^n xy^2 + 2^\alpha \times (11 \times 3^n + 3n - 6)x^2y^2 + 4^\alpha \times (12 \times 3^n - 4)x^2y^4, \\
D_x^\alpha D_y^\alpha(f(x, y)) &= 6 \times 2^\alpha \times 3^n xy^2 + 4^\alpha \times (11 \times 3^n + 3n - 6)x^2y^2 + 8^\alpha \times (12 \times 3^n - 4)x^2y^4.
\end{aligned} \tag{12}$$

Using the derived formulas of M -polynomial given in Table 1, we find

- (1) $M_1(G) = (D_x + D_y)(f(x, y))|_{x=y=1} = 134 \times 3^n + 12n - 48$
- (2) $M_2(G) = D_x D_y(f(x, y))|_{x=y=1} = 152 \times 3^n + 12n - 56$
- (3) ${}^m M_2(G) = S_x S_y(f(x, y))|_{x=y=1} = (29/4) \times 3^n + (3/4)n - 2$
- (4) $R(G) = D_x^\alpha D_y^\alpha(f(x, y))|_{x=y=1}, \alpha = -1/2 = (6\sqrt{2} + (11/2)) \times 3^n + (3/2)n - (3 + \sqrt{2})$ $\square$

Theorem 3. Let G be the PEG-cored triazine dendrimer. Then, the M -polynomial for G is given as

$$M(C_{60}, x, y) = 6 \times 3^n x y^2 + (11 \times 3^n + 3n - 6)x^2 y^2 + (12 \times 3^n - 4)x^2 y^4. \quad (13)$$

Proof. There are three types of edge partitions based on degrees of end vertices of each edge for the PEG-cored triazine dendrimer. The first edge partitions E_{12} contains 8×4^n edges, where $d_u = 1$ and $d_v = 2$. The second edge partition E_{22} contains $1/3(40 \times 4^n + 9n - 19)$ edges, where

$d_u = d_v = 2$. The third edge partition E_{23} contains $(24 \times 4^n - 6)$ edges, where $d_u = 2$ and $d_v = 3$.

Therefore, the M -polynomial of G is

$$M(G, x, y) = \sum_{i \leq j} m_{ij} x^i y^j = 8 \times 4^n x y^2 + \frac{1}{3}(40 \times 4^n + 9n - 19)x^2 y^2 + (24 \times 4^n - 6)x^2 y^3. \quad (14)$$

$\square$

Proposition 3. The first Zagreb index $M_1(G)$, the second Zagreb index $M_2(G)$, second modified Zagreb index ${}^m M_2(G)$, and the general Randić index $R_\alpha(G)$, where $\alpha \in \mathbb{N}$, for the PEG-cored triazine dendrimer G are given as

- (1) $M_1(G) = (529/3) \times 4^n + 12n - (166/3)$
- (2) $M_2(G) = (640/3) \times 4^n + 12n - (184/3)$
- (3) ${}^m M_2(G) = (34/3) \times 4^n + (3/4)n - (31/12)$
- (4) $R(G) = ((8/\sqrt{2}) + (24/\sqrt{6}) + (20/3)) \times 4^n + (3/2)n - ((19/6) + (6/\sqrt{6}))$

Proof. Let $f(x, y)$ be the M -polynomial of G . Then,

$$\begin{aligned} D_x(f(x, y)) &= 8 \times 4^n x y^2 + \frac{2}{3}(40 \times 4^n + 9n - 19)x^2 y^2 + 2(24 \times 4^n - 6)x^2 y^3, \\ D_y(f(x, y)) &= 16 \times 4^n x y^2 + \frac{2}{3}(40 \times 4^n + 9n - 19)x^2 y^2 + 3(24 \times 4^n - 6)x^2 y^3, \\ D_x D_y(f(x, y)) &= 16 \times 4^n x y^2 + \frac{4}{3}(40 \times 4^n + 9n - 19)x^2 y^2 + 6(24 \times 4^n - 6)x^2 y^3, \\ S_y(f(x, y)) &= 4 \times 4^n x y^2 + \frac{1}{6}(40 \times 4^n + 9n - 19)x^2 y^2 + (8 \times 4^n - 2)x^2 y^3, \\ S_x S_y(f(x, y)) &= 4 \times 4^n x y^2 + \frac{1}{12}(40 \times 4^n + 9n - 19)x^2 y^2 + (4 \times 4^n - 1)x^2 y^3, \\ D_y^\alpha(f(x, y)) &= 8 \times 2^\alpha \times 4^n x y^2 + \frac{2^\alpha}{3}(40 \times 4^n + 9n - 19)x^2 y^2 + 3^\alpha(24 \times 4^n - 6)x^2 y^3, \\ D_x^\alpha D_y^\alpha(f(x, y)) &= 8 \times 2^\alpha \times 4^n x y^2 + \frac{4^\alpha}{3}(40 \times 4^n + 9n - 19)x^2 y^2 + 6^\alpha(24 \times 4^n - 6)x^2 y^3. \end{aligned} \quad (15)$$

Using the derived formulas of M -polynomial given in Table 1, we find

- (1) $M_1(G) = (D_x + D_y)(f(x, y))|_{x=y=1} = (529/3) \times 4^n + 12n - (166/3)$
- (2) $M_2(G) = D_x D_y(f(x, y))|_{x=y=1} = (640/3) \times 4^n + 12n - (184/3)$
- (3) ${}^m M_2(G) = S_x S_y(f(x, y))|_{x=y=1} = (34/3) \times 4^n + (3/4)n - (31/12)$

$$(4) R(G) = D_x^\alpha D_y^\alpha(f(x, y))|_{x=y=1, \alpha=-1/2} = ((8/\sqrt{2}) + (24/\sqrt{6}) + (20/3)) \times 4^n + (3/2)n - ((19/6) + (6/\sqrt{6})) \quad \square$$

4. Conclusion

Chemical graph theory plays an important role in studying the molecular structure of the chemical compounds. Calculating the topological indices of the chemical structure using graph theory is important to study the large amount of

information about their physical properties. In this study, we derive the M -polynomials for the PEG-cored PAMAM, carbosilane, and poly (lysine) dendrimers and calculate their first, second, and second modified Zagreb indices and the Randić index. This work may provide the role in determining the properties of these dendrimeric structures.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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