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# Some degree-based topological indices of caboxy-terminated dendritic macromolecule

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**Abstract:** In the modern era of the chemical science, the chemical graph theory has contributed significantly to exploring the properties of the chemical compounds. Currently, the computation of the topological indices is one of the most active directions of the research in the area of the chemical graph theory. The main feature of the study of the topological indices is its its ability of predicting the various physio-chemical properties. In this article, we compute several degree-based topological indices for the caboxy-terminated dendritic macromolecule. We compute Harmonic index, atom-bond connectivity index, geometric arithmetic index, sum connectivity index, inverse sum index, symmetric division degree, and Zagreb indices for caboxy-terminated dendritic macromolecule. The obtained results have potential to predict biochemical properties such as viscosity, entropy, and boiling point.

**Keywords:** molecular graphs, topological index, degree of vertex

## 1 Introduction

The recent impact of the graph theory in the field of chemistry highlights the importance of the cheminformatics, which deals with the chemistry, information sciences, and mathematics. A lot of research has already been done in this direction during the last few years. For a molecule, the chemical structural study is done by using its molecular graph. In a molecular graph, the atoms and bonds of a chemical structure are represented by the vertices and the edges, respectively. We use standard notations from the field of the graph theory such as: we denote a graph with vertex set $V$ and an edge set $E$ by $G(V, E)$ or $G$ and the degree of a vertex $v$ by $d_v$.

In 1947, Wiener, while studying boiling point of alkane, introduced a numerical invariant called Wiener index (Wiener, 1947). Wiener index approximates the boiling point of hydrocarbon molecules. Due to its applicability, more topological indices (invariants) have been defined over the last few decades, which are useful in approximating the biochemical properties of molecular structures. The study of the topological indices associated to molecular graphs made a significant contribution in understanding their chemical and physical properties.

Before proceeding further, we recall the notions of few well-known topological indices.

In 1987, Fajtlowicz introduced an index called harmonic index (Fajtiowicz, 1987), defined as:

$$H(G) = \sum_{uv\in E(G)} \frac{2}{d_u+d_v} \tag{1}$$

Atom bond connectivity index was introduced in Estrada et al. (1998). It is defined as follows:

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \tag{2}$$

The geometric arithmetic index was introduced in Vukicevic and Furtula (2009) is defined as:

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \tag{3}$$

The sum connectivity index was introduced in Zhou and Trinajstic (2009), which is given by the formula:

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u+d_v}} \tag{4}$$

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In 2010, two more topological indices were introduced by Vukicevic and Gasperov (2010) and Vukicevic (2010), which are named inverse sum index and symmetric division degree index, respectively:

$$ISI(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v} \tag{5}$$

$$SDD(G) = \sum_{uv \in E(G)} \left[\frac{\min\ (d_u, d_v)}{\max\ (d_u, d_v)} + \frac{\max\ (d_u, d_v)}{\min\ (d_u, d_v)}\right] \tag{6}$$

Furtula and Gutman (2015) introduced the following topological index, known as forgotten topological index:

$$F(G) = \sum_{uv \in E(G)} [(d_u)^2 + (d_v)^2] \tag{7}$$

Moreover, the topological polynomial associated to the forgotten topological index is defined as $F$-polynomial:

$$mF(G, x) = \sum_{uv \in E(G)} x^{[(d_u)^2 + (d_v)^2]} \tag{8}$$

Another class of the degree-based topological indices are Zagreb indices. The first and the second Zagreb indices were introduced by Gutman and Trinajstic (1972) as:

$$M_1(G) = \sum_{u \in V(G)} (d_u)^2 = \sum_{uv \in E(G)} d_u + d_v \tag{9}$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v \tag{10}$$

The corresponding polynomials are defined as:

$$M_1(G, x) = \sum_{uv \in E(G)} x^{d_u + d_v} \tag{11}$$

and

$$M_2(G, x) = \sum_{uv \in E(G)} x^{d_u d_v} \tag{12}$$

The modified forms of the first and the second Zagreb indices were introduced by Milicevic, Nikolic, and Trinajstic (Milicevic et al., 2004) as:

$$^{m}M_1(G) = \sum_{uv \in E(G)} \frac{1}{(d_u)^2} \tag{13}$$

$$^{m}M_2(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v} \tag{14}$$

The multiplicative version of the first and the second Zagreb indices were introduced by Gutman (2011), as follows:

$$\prod_1(G) = \prod_{u \in V(G)} (d_u)^2 \tag{15}$$

$$\prod_2(G) = \prod_{uv \in E(G)} (d_u d_v) \tag{16}$$

The augmented Zagreb index (Furtula et al., 2010) and the hyper Zagreb index (Shirdel et al., 2013) were introduced in 2010 and 2013, respectively, as follows:

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3 \tag{17}$$

$$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2 \tag{18}$$

These indices have been computed already for many molecular structures. For comprehensive overview related to topological indices and their recent applications, we refer the readers to Ahmad et al. (2019), Alfuraidan et al. (2020), Alsharafi et al. (2020), Bashir et al. (2017), Fahad et al. (2021a, 2021b), Hussain et al. (2019), Jalil et al. (2020), Jamil et al. (2020), Munir et al. (2017), Nadeem et al. (2020), Patil and Yattinahalli (2020), Shabir et al. (2020), Ye et al. (2019), Zhang et al. (2020), Zhao et al. (2019), and Zheng et al. (2019).

On the other hand, the water solvable acid has many benefits, for example pantothenic acid is used in the food supplements and helps in digestion of food. The water solvable pesticides are useful in the sense that their molecules bond with the molecules of water and travel long with the water. The PAMAM dendrimers are the most studied dendrimers due to their solvability in most of the solvents, particularly water. A macromolecule, named as carboxy-terminated dendritic macromolecule $\{(HO_2C)_{2^n} - [G - n]\}_2.[C]$, obtained by the chemical reaction carried out to increase the water solvability of polyacid (Hawker et al., 1993) is shown in Figure 1. The detailed study of the reaction scheme for the preparation of caboxy-terminated dendritic macromolecule can be seen in Hawker et al. (1993). By keeping in view its property of water solvability, we compute all the topological indices described above. Moreover, we also analyze the obtained results by using the graphical tools.

## 2 Degree-based indices of carboxy-terminated dendritic macromolecule

In this section, we compute some degree-based topological indices for the caboxy-terminated dendritic macromolecule. From now onward, $G = G(V, E)$ denotes the molecular graph of caboxy-terminated dendritic macromolecule with the termination at th growth. It is easy to verify that $|V(G)| = 38 \times 2^n - 4$ and $|E(G)| = 42 \times 2^n - 5$.

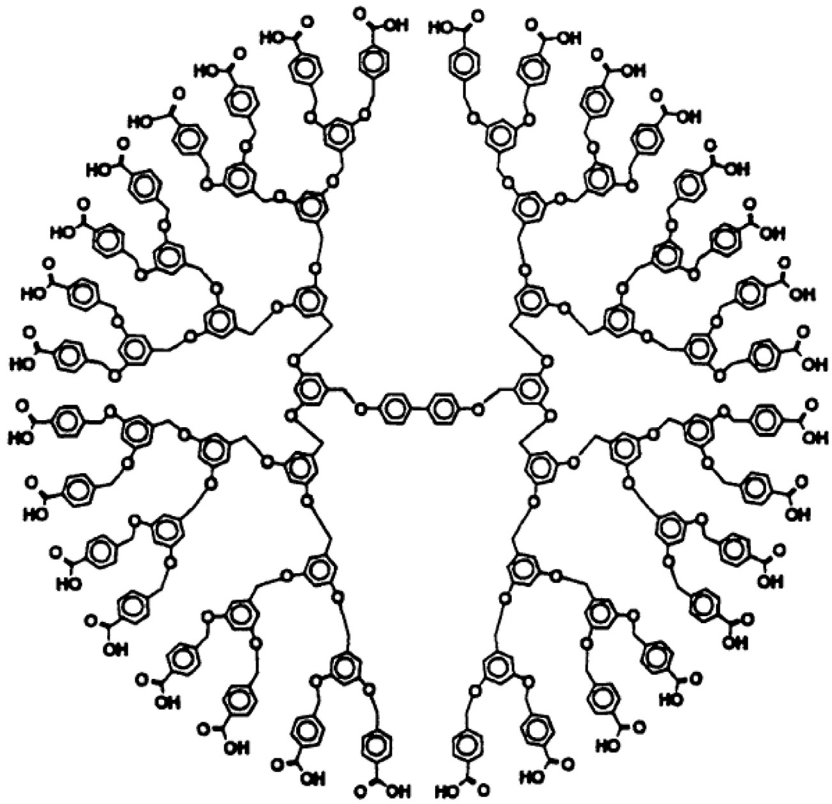


**Figure 1:** Carboxy-terminated dendritic macromolecule for $n = 4$.

In order to prove our results, we partitioned the set of edges on the bases of degrees of the end vertices of edges, as $E_{1,3}(G)$, $E_{2,2}(G)$, $E_{2,3}(G)$ and $E_{3,3}(G)$ as follows:

$$E_{1,3}(G) = \{uv \in E(G): d_u = 1, d_v = 3\}$$
$$E_{2,2}(G) = \{uv \in E(G): d_u = 2, d_v = 2\}$$
$$E_{2,3}(G) = \{uv \in E(G): d_u = 2, d_v = 3\}$$
$$E_{3,3}(G) = \{uv \in E(G): d_u = 3, d_v = 3\}$$

From the Figure 1, we obtained Table 1.

Now, the above information yields the following results.

**Table 1:** Number of edges in each set of partition

| Edge set | Number of edges |
|---|---|
| $E_{1,3}(G)$ | $4 \times 2^n$ |
| $E_{2,2}(G)$ | $8 \times 2^n + 2$ |
| $E_{2,3}(G)$ | $28 \times 2^n - 8$ |
| $E_{3,3}(G)$ | $2 \times 2^n + 1$ |

**Theorem 1**
Let Let $G$ be the molecular graph of caboxy-terminated dendritic macromolecule and $n \geq 1$, we have:

1) $H(G) = \frac{134}{15} \times 2^{n+1} - \frac{28}{15}$
2) $ABC(G) = 2^{n+1}\left(2\sqrt{\frac{2}{3}} + 18\sqrt{\frac{1}{2}} + \sqrt{\frac{4}{9}}\right) + \sqrt{\frac{4}{9}} - 6\sqrt{\frac{1}{2}}$
3) $GA(G) = 2^{n+1}\left(\sqrt{3} + \frac{28\sqrt{6}}{5} + 5\right) + 3 - \frac{16\sqrt{6}}{5}$
4) $\chi(G) = 2^{n+1}\left(3 + \frac{14}{\sqrt{5}} + \frac{1}{\sqrt{6}}\right) + 1 - \frac{8}{\sqrt{5}} - \frac{1}{\sqrt{6}}$
5) $ISI(G) = \frac{119}{5} \times 2^{n+1} - \frac{61}{10}$
6) $SDD(G) = 47 \times 2^{n+1} - \frac{34}{3}$
7) $F(G) = 252 \times 2^{n+1} - 70$

*Proof.* By using the Table 1 and definition of the topological indices, we have:

$$H(G) = 4 \times 2^n\left(\frac{2}{1+3}\right) + (8 \times 2^n + 2)\left(\frac{2}{2+2}\right) + (28 \times 2^n - 8)\left(\frac{2}{2+3}\right) + (2 \times 2^n + 1)\left(\frac{2}{3+3}\right)$$

$$= 4 \times 2^n\left(\frac{1}{2}\right) + (8 \times 2^n + 2)\left(\frac{1}{2}\right) + (28 \times 2^n - 8)\left(\frac{2}{5}\right) + (2 \times 2^n + 1)\left(\frac{1}{3}\right)$$

$$= 2 \times 2^n \left(1 + 2 + \frac{28}{5} + \frac{1}{3}\right) - \frac{28}{15}$$

$$= \frac{134}{15} \times 2^{n+1} - \frac{28}{15}.$$

$$ABC(G) = 4 \times 2^n \sqrt{\frac{1+3-2}{1 \times 3}} + (8 \times 2^n + 2)\sqrt{\frac{2+2-2}{2 \times 2}}$$

$$+ (28 \times 2^n - 8)\sqrt{\frac{2+3-2}{2 \times 3}}$$

$$+(2 \times 2^n + 1)\sqrt{\frac{3+3-2}{3 \times 3}}$$

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

$$+ (28 \times 2^n - 8)\sqrt{\frac{3}{6}} + (2 \times 2^n + 1)\sqrt{\frac{4}{9}}$$

$$= 2^{n+1}\left(2\sqrt{\frac{2}{3}} + 18\sqrt{\frac{1}{2}} + \sqrt{\frac{4}{9}}\right) + \sqrt{\frac{4}{9}} - 6\sqrt{\frac{1}{2}}$$

$$GA(G) = 4 \times 2^n \left(2\frac{\sqrt{1 \times 3}}{1+3}\right) + (8 \times 2^n + 2)\left(2\frac{\sqrt{2 \times 2}}{2+2}\right)$$

$$+ (28 \times 2^n - 8)\left(2\frac{\sqrt{2 \times 3}}{2+3}\right)$$

$$+ (2 \times 2^n + 1)\left(2\frac{\sqrt{3 \times 3}}{3+3}\right)$$

$$= 4 \times 2^n \left(2\frac{\sqrt{3}}{4}\right) + (8 \times 2^n + 2)(1)$$

$$+ (28 \times 2^n - 8)\left(2\frac{\sqrt{6}}{5}\right) + (2 \times 2^n + 1)(1)$$

$$= 2^{n+1}\left(\sqrt{3} + \frac{28\sqrt{6}}{5} + 5\right) + 3 - \frac{16\sqrt{6}}{5}$$

$$\chi(G) = 4 \times 2^n \frac{1}{\sqrt{1+3}} + (8 \times 2^n + 2)\frac{1}{\sqrt{2+2}}$$

$$+ (28 \times 2^n - 8)\frac{1}{\sqrt{2+3}} + (2 \times 2^n + 1)\frac{1}{\sqrt{3+3}}$$

$$= 4 \times 2^n \frac{1}{2} + (8 \times 2^n + 2)\frac{1}{2} + (28 \times 2^n - 8)\frac{1}{\sqrt{5}}$$

$$(2 \times 2^n + 1)\frac{1}{\sqrt{6}}$$

$$= 2^{n+1}\left(3 + \frac{14}{\sqrt{5}} + \frac{1}{\sqrt{6}}\right) + 1 - \frac{8}{\sqrt{5}} - \frac{1}{\sqrt{6}}$$

$$ISI(G) = 4 \times 2^n \frac{1 \times 3}{1+3} + (8 \times 2^n + 2)\frac{2 \times 2}{2+2}$$

$$+ (28 \times 2^n - 8)\frac{2 \times 3}{2+3} + (2 \times 2^n + 1)\frac{3 \times 3}{3+3}$$

$$= 2^{n+1} \times \left(\frac{3}{2} + \frac{3}{2} + \frac{84}{5} + 4\right) - \frac{61}{10}$$

$$= \frac{119}{5} \times 2^{n+1} - \frac{61}{10}$$

$$SDD(G) = 4 \times 2^n \left(\frac{1}{3} + \frac{3}{1}\right) + (8 \times 2^n + 2)\left(\frac{2}{2} + \frac{2}{2}\right)$$

$$+ (28 \times 2^n - 8)\left(\frac{2}{3} + \frac{3}{2}\right)$$

$$+ (2 \times 2^n + 1)\left(\frac{3}{3} + \frac{3}{3}\right)$$

$$= 2 \times 2^{n+1}\left(\frac{10}{3} + 5 + \frac{91}{6}\right) - \frac{34}{3}$$

$$= 47 \times 2^{n+1} - \frac{34}{3}$$

$$F(G) = 4 \times 2^n((1)^2 + (3)^2)$$

$$+ (8 \times 2^n + 2)((2)^2 + (2)^2)$$

$$+ (28 \times 2^n - 8)((2)^2 + (3)^2)$$

$$+(2 \times 2^n + 1)((3)^2 + (3)^2)$$

$$= 2 \times 2^{n+1}(2(10) + 4(8) + 14(13) + 18) - 70$$

$$= 252 \times 2^{n+1} - 70$$

Which completes the proof.

**Theorem 2**
Let $G$ be the molecular graph of caboxy-terminated dendritic macromolecule and $n \geq 1$, then the $F$–polynomial is given as:

$$mF(G,x) = 4 \times 2^n x^{10} + (8 \times 2^n + 2)x^8 + (28 \times 2^n - 8)x^{13} + (2 \times 2^n + 1)x^{18}$$

*Proof.* Follows from the Table 1 and Eq. 8.

Now, we present the comparison of the obtained results by using the Table 2 and analyzing the values graphically, see Figure 2.

Clearly, it can be seen that the behavior of indices is toward rise.

**Table 2:** Comparison table for degree-based indices

| Index | $n = 1$ | $n = 2$ | $n = 3$ | $n = 4$ | $n = 5$ |
|---|---|---|---|---|---|
| $H(G)$ | 33.866 | 69.600 | 141.066 | 284.000 | 569.866 |
| $\chi(G)$ | 35.690 | 74.367 | 151.721 | 306.429 | 615.845 |
| $ABC(G)$ | 56.534 | 116.644 | 236.865 | 477.306 | 958.189 |
| $GA(G)$ | 76.958 | 158.755 | 322.348 | 649.535 | 1303.910 |
| $ISI(G)$ | 89.100 | 184.300 | 374.700 | 755.500 | 1517.100 |
| $SDD(G)$ | 176.666 | 364.666 | 740.666 | 1492.666 | 2996.666 |
| $F(G)$ | 938.000 | 1946.000 | 3962.000 | 7994.000 | 16058.000 |

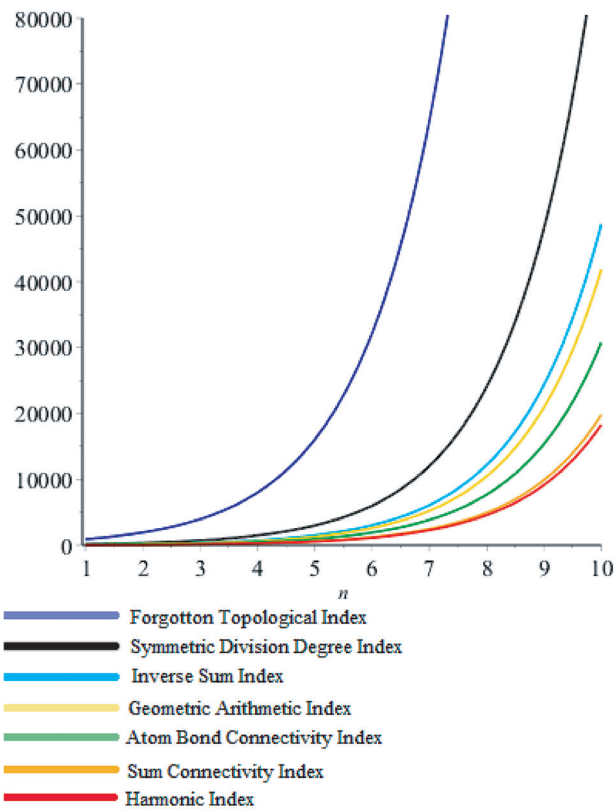


**Figure 2:** Comparison of degree-based indices.

## 3 Zagreb indices of caboxy-terminated dendritic macromolecule

In this section, we compute some Zagreb topological indices for the caboxy-terminated dendritic macromolecule. We partitioned the set of vertices $V(G)$ on the bases of degree of vertices in to the following subsets $V_1(G)$, $V_2(G)$ and $V_3(G)$, which consists of vertices of degree 1, 2, and 3, respectively.

**Table 3:** Number of vertices in each set of vertex partition

| Vertex set | Number of vertices |
|---|---|
| $V_1(G)$ | $4 \times 2^n$ |
| $V_2(G)$ | $22 \times 2^n - 2$ |
| $V_3(G)$ | $12 \times 2^n - 2$ |

Now, we prove the following theorem.

**Theorem 3**
Let Let $G$ be the molecular graph of caboxy-terminated dendritic macromolecule and $n \geq 1$, we have:

1) $M_1(G) = 200 \times 2^n - 26$
2) $M_2(G) = 230 \times 2^n - 31$
3) ${}^mM_1(G) = \frac{65}{6}2^n - \frac{13}{18}$
4) ${}^mM_2(G) = \frac{74}{9}2^n - \frac{13}{18}$
5) $\prod_1(G) = 4^{(22\times 2^n - 2)} \times 9^{(12\times 2^n - 2)}$
6) $\prod_2(G) = 3^{(4\times 2^n)} \times 9^{(8\times 2^n + 2)} \times 4^{(28\times 2^n - 8)} \times 9^{(2\times 2^n + 1)}$
7) $AZI(G) = \frac{10377}{32} \times 2^n - \frac{2343}{64}$
8) $HM(G) = 964 \times 2^n - 132$

*Proof.* By using the Tables 1 and 3 and the definitions of indices, we have:

$$\begin{aligned} M_1(G) &= 4 \times 2^n(1)^2 + (22 \times 2^n - 2)(2)^2 \\ &\quad + (12 \times 2^n - 2)(3)^2 \\ &= 200 \times 2^n - 26 \\ M_2(G) &= 4 \times 2^n(1 \times 3) + (8 \times 2^n + 2)(2 \times 2) \\ &\quad + (28 \times 2^n - 8)(2 \times 3) + (2 \times 2^n + 1)(3 \times 3) \\ &= 230 \times 2^n - 31 \\ {}^mM_1(G) &= 4 \times 2^n \frac{1}{(1)^2} + (22 \times 2^n - 2)\frac{1}{(2)^2} \\ &\quad + (12 \times 2^n - 2)\frac{1}{(3)^2} \\ &= \frac{65}{6}2^n - \frac{13}{18} \end{aligned}$$

**Table 4:** Comparison table for Zagreb indices

| Index | $n = 1$ | $n = 2$ | $n = 3$ | $n = 4$ | $n = 5$ |
|---|---|---|---|---|---|
| $^mM_2(G)$ | 15.722 | 32.166 | 65.055 | 130.833 | 262.388 |
| $^mM_1(G)$ | 20.944 | 42.611 | 85.944 | 172.611 | 345.944 |
| $M_1(G)$ | 374.000 | 774.000 | 1574.000 | 3174.000 | 6374.000 |
| $M_2(G)$ | 429.000 | 889.000 | 1809.000 | 3649.000 | 7329.000 |
| $AZI(G)$ | 611.953 | 1260.515 | 2557.640 | 5151.890 | 10340.390 |
| $HM(G)$ | 1796.000 | 3724.000 | 7580.000 | 15292.000 | 30716.000 |

$$
\begin{aligned}
{}^mM_2(G) &= 4\times 2^n \tfrac{1}{1\times 3} + (8\times 2^n + 2)\tfrac{1}{2\times 2} \\
&\quad + (28\times 2^n - 8)\tfrac{1}{2\times 3} + (2\times 2^n + 1)\tfrac{1}{3\times 3} \\
&= \frac{74}{9}2^n - \frac{13}{18}
\end{aligned}
$$

$$
\begin{aligned}
\prod\nolimits_1(G) &= \underbrace{1^2\times\ldots\times 1^2}\times\underbrace{2^2\times\ldots\times 2^2}\times\underbrace{3^2\times\ldots\times 3^2} \\
&= 1^{(4\times 2^n)}\times 4^{(22\times 2^n - 2)}\times 9^{(12\times 2^n - 2)} \\
&= 4^{(22\times 2^n - 2)}\times 9^{(12\times 2^n - 2)}
\end{aligned}
$$

$$
\begin{aligned}
\prod\nolimits_1(G) &= \underbrace{3\times\ldots\times 3}\times\underbrace{4\times\ldots\times 4}\times\underbrace{6\times\ldots\times 6}\times\underbrace{9\times\ldots\times 9} \\
&= 3^{(4\times 2^n)}\times 4^{(8\times 2^n + 2)}\times 6^{(28\times 2^n - 8)}\times 9^{(2\times 2^n + 1)}
\end{aligned}
$$

$$
\begin{aligned}
AZI(G) &= 4\times 2^n\left(\frac{1\times 3}{1+3-2}\right)^3 \\
&\quad + (8\times 2^n + 2)\left(\frac{2\times 2}{2+2-2}\right)^3 \\
&\quad + (28\times 2^n - 8)\left(\frac{2\times 3}{2+3-2}\right)^3 \\
&\quad + (2\times 2^n + 1)\left(\frac{3\times 3}{3+3-2}\right)^3 \\
&= 4\times 2^n\left(\frac{27}{8}\right) + (8\times 2^n + 2)(8) \\
&\quad + (28\times 2^n - 8)\left(\frac{216}{27}\right) + (2\times 2^n + 1)\left(\frac{729}{64}\right) \\
&= \frac{10377}{32}\times 2^n - \frac{2343}{64}
\end{aligned}
$$

$$
\begin{aligned}
HM(G) &= 4\times 2^n(1+3)^2 + (8\times 2^n + 2)(2+2)^2 \\
&\quad + (28\times 2^n - 8)(2+3)^2 \\
&\quad + (2\times 2^n + 1)(3+3)^2 \\
&= 4\times 2^n(16) + (8\times 2^n + 2)(16) \\
&\quad + (28\times 2^n - 8)(25) + (2\times 2^n + 1)(36) \\
&= 964\times 2^n - 132
\end{aligned}
$$

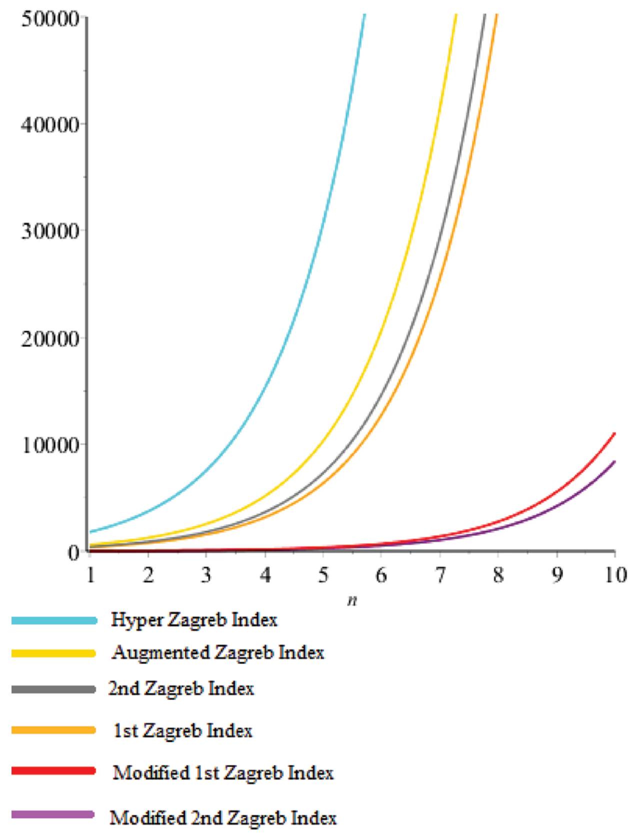


**Figure 3:** Comparison of Zagreb indices.

**Theorem 4**
Let Let $G$ be the molecular graph of caboxy-terminated dendritic macromolecule and $n \geq 1$, then the first and second Zagreb polynomials are given as:

$$
\begin{aligned}
M_1(G,x) &= 4\times 2^n x^4 + (8\times 2^n + 2)x^4 \\
&\quad + (28\times 2^n - 8)x^5 + (2\times 2^n + 1)x^6
\end{aligned}
$$

$$
\begin{aligned}
M_2(G,x) &= 4\times 2^n x^3 + (8\times 2^n + 2)x^4 \\
&\quad + (28\times 2^n - 8)x^6 + (2\times 2^n + 1)x^9
\end{aligned}
$$

*Proof.* The proof follows from the Table 1 and the definitions given in Eq. 11 and 12.

To conclude the section, we present the comparison of the topological indices by using the Table 4 and graphical analysis, see Figure 3.

The graph indicates that, the Zagreb indices are in the increasing behaviour.

## 4 Conclusion

In this article, we studied the molecular graph of caboxy-terminated dendritic macromolecule. We computed the harmonic index, atom bond connectivity index, geometric arithmetic index, sum connectivity index, symmetric division degree index, inverse sum index, forgotten topological index, the first and the second Zagreb indices, modified forms of the first and the second Zagreb indices, multiplicative version of the first and the second Zagreb indices, augmented Zagreb index, and hyper Zagreb index. Also associated polynomials of forgotten topological index, the first and the second Zagreb indices are given. Beside these, we have presented the graphical analysis (Figures 2 and 3) and comparison tables (Tables 2 and 4). Our computed results may play a vital role in visualizing the topology of the molecular structure of caboxy-terminated dendritic macromolecule.

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