Multiplicative degree based topological indices of some chemical structures in drug

Murat Cancan¹ orcid.org/0000-0002-8606-2274

Sourav Mondal² orcid.org/0000-0003-1928-7075

Nilanjan De³ orcid.org/0000-0001-9143-7045

Anita Pal⁴ orcid.org/0000-0002-2514-5463

¹Van Yüzüncü Yıl University, Faculty of Education, Van, Turkey.

✉ mcancan@yyu.edu.tr

National Institute of Technology Durgapur, Dept. of mathematics, Durgapur, WB, India.

²✉ souravmath94@gmail.com; ⁴✉ anita.buie@gmail.com

³Calcutta Institute of Engineering & Management, Dept. of Basic Sci and Humanities, WB, Kolkata, India.

✉ de.nilanjan@rediffmail.com

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Abstract:

In quantitative structure property relationship analysis (QSPR) and quantitative structure property relationship analysis (QSAR) the correlation between different properties/activities and molecular structure of chemical compounds is investigated which is helpful in drug design. Topological index is an useful tool to predict different physical and chemical properties of molecule by collecting information from the molecular graph. In this article, multiplicative degree based topological indices are obtained for some chemical structures widely used in drug design, especially in anticancer drug discovery. To visualize the indices, the results are interpreted graphically.

Keywords: Topological index; Dox-loaded micelle comprising PEGPasp block copolymer with chemically conjugated Dox SP[n]; Polyomino chain of n-cycles; Triangular benzenoid (T_n); Circumcoronene benzenoid series (H_k).

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1. Introduction

With rapid development in chemical field, it is very difficult to perform chemical experiments which increase cost and time to determine properties of particular compound. So, a new technique called chemical graph theory evolved. The chemical graph theory is one of the most popular subjects in the field of graph theory. In chemical graph theory, we deal with molecular graph [1], a simple connected graph, to determine physiochemical and psychochemical properties of particular compound. In this field of research, topological index plays a prominent role to study the topological properties of different chemical structures. Topological index is a numerical parameter associated with the molecular graph of chemical compound. It remains unchanged under graph isomorphism. Now a days lot of research work is presented in chemical graph theory particularly in investigating topological properties of chemically significant composite graphs. Gao et al. [2] have derived degree based topological indices for the family of smart polymers which is widely used in anticancer drugs manufacturing. Kwun et al. [3] obtained multiplicative degree based topological indices of some silicon-carbon structures. Topological properties of some chemical structures used in drug design have been studied in [4, 5]. For more works on this field, readers are referred to [6, 7, 8, 9, 10, 11, 12]. In this paper we have computed some multiplicative degree based topological indices of chemical compounds widely used in drug discovery, especially, the family of smart polymers to produce anticancer drugs which is a modern topic of research in medical science. Further, we have considered polyomino chain of n -cycle, triangular benzenoid (T_n) and circumcoronene benzenoid series (H_k).

2. Some basic definitions

Throughout this paper, we consider simple connected graph. Let $V(G)$ and $E(G)$ be the vertex and edge sets of a graph G , respectively. The degree of a vertex $v \in V(G)$, denoted by $d(v)$, is the count of edges incident to v . The cycle graph with n nodes is denoted by C_n . Wang et al. defined a general multiplicative index [13] as follows:

$$(2.1) \quad W_1^s(G) = \prod_{u \in V(G)} (d(u))^s.$$

Where s is real number. For $s = 1, 2$, in (2.1), the Narumi-Katayama

index [14] and the first multiplicative Zagreb index [15] are defined respectively, as follows:

$$NK(G) = \prod_{u \in V(G)} d(u), \quad \Pi_1(G) = \prod_{u \in V(G)} (d(u))^2.$$

Kulli et al. introduced two more indices known as first and second generalized multiplicative Zagreb indices [16] which are defined as follows:

$$(2.2) \quad MZ_1^a(G) = \prod_{uv \in E(G)} (d(u) + d(v))^a,$$

$$(2.3) \quad MZ_2^a(G) = \prod_{uv \in E(G)} (d(u)d(v))^a.$$

Where a is real number. Considering $a = 1, 2, -1/2$ in (2.2), new version of the multiplicative first Zagreb index [17], first multiplicative hyper-Zagreb index [18], multiplicative sum connectivity index [19] are defined respectively, as follows:

$$\Pi_1^*(G) = \prod_{uv \in E(G)} (d(u) + d(v)), \quad H\Pi_1(G) = \prod_{uv \in E(G)} (d(u) + d(v))^2,$$

$$SC\Pi(G) = \prod_{uv \in E(G)} (d(u) + d(v))^{-\frac{1}{2}}.$$

Putting $a = 1, 2, -\frac{1}{2}$ in (2.3), second multiplicative Zagreb index [15], second multiplicative hyper-Zagreb index [18], and multiplicative product connectivity index [19] are defined respectively as follows:

$$\Pi_2(G) = \prod_{uv \in E(G)} d(u)d(v), \quad H\Pi_2(G) = \prod_{uv \in E(G)} (d(u)d(v))^2,$$

$$PC\Pi(G) = \prod_{uv \in E(G)} (d(u)d(v))^{-\frac{1}{2}}.$$

Multiplicative atomic bond connectivity index and multiplicative Geometric arithmetic index are defined [3] respectively as follows:

$$ABC(G) = \prod_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}, \quad GAH(G) = \prod_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}.$$

3. Motivation

Smart polymers are composed of high performance polymers that change its physiochemical properties according to the environment they are in. Thus smart polymers are stimuli-responsive polymers. Polymeric micelles are most accepted modalities of macro-molecular drug delivery systems. It gives unique effect on body for drug targeting, tumor accumulation. Polymeric micelle has advantages such as controlled drug release, high drug loading capacity, unnecessariness of chemical structure modification of the drug etc [20]. PEG is widely used hydrophilic polymer for drug delivery. The hydrated PEG shell increase stability and enhance blood flow times of drug that is protected by or bound to PEG. The Polymer, PEG-b-PASP-DOX conjugation has been accomplished by means of acid cleavable hydrazones linkages [21]. Over the past few years, polymeric micelles of DOX conjugated poly (ethylene glycol)-b-poly (aspirate) (PEG-b-PASP) block copolymers have gained considerable attention because of their ease in the formation of micelles in water [22]. The Dox-loaded micelle containing PEG-PAsp block copolymer with chemically conjugated Dox ($SP[n]$), depicted in Figure 3.1, is a famous family of smart polymer which is used as anthracycline anticancer antibiotic and applied in treating various kinds of cancers.

Figure 3.1: Chemical structure of $SP[n]$.

Figure 3.2: The zig-zag chain of 8-cycles.

A polyomino system is a finite 2-connected planar graph so that a regular C_4 cycle of length one surrounds the internal cell. In polyomino system two nodes are adjacent iff two cells share a common edge [23]. Its structure is depicted in Figure 3.2. Polyomino systems have several applications in crystal physics [24]. We also consider graph of triangular benzenoid T_n in which n is number of hexagonal structure in base graph. We clearly observe from Figure 3.3 that T_n has $\frac{1}{2}n(n+1)$ hexagons [25]. Circumcoronene benzenoid series consist of several copies of benzene C_6 on the perimeter (Figure 3.5,3.4). After generalization from benzene molecules we get the circumcoronene series of benzenoid. Benzene is important from chemistry point of view as it helps in formation of aromatic compound.

4. Main Results

In this section, we focus on computing the multiplicative degree based topological indices of the molecular graphs discussed in the previous section.

4.1. Multiplicative topological indices of Dox-loaded micelle comprising PEG-PAsp block copolymer with chemically conjugated Dox ($SP[n]$)

Figure 3.3: Molecular graph of triangular benzenoid.

Theorem 1. Let G be the Dox-loaded micelle comprising PEG-PAsp block copolymer with chemically conjugated Dox ($SP[n]$). Then we have

- (i) $W_1^s(G) = 2^{s(18n+4)} \cdot 3^{(20ns)}$,
- (ii) $MZ_1^a(G) = 2^{2a(23n+5)} \cdot 3^{a(20n+1)} \cdot 5^{a(19n-1)} \cdot 7^{(an)}$,
- (iii) $MZ_2^a(G) = 2^{8a(5n+1)} \cdot 3^{(60an)}$,
- (iv) $ABC(G) = \left(\frac{1}{\sqrt{2}}\right)^{(27n+4)} \cdot \left(\sqrt{\frac{2}{3}}\right)^{(9n+1)} \cdot \left(\frac{\sqrt{3}}{2}\right)^{(n)} \cdot \left(\frac{4}{5}\right)^{(n)} \cdot \left(\frac{2}{3}\right)^{(16n)} \cdot \left(\frac{\sqrt{5}}{2\sqrt{3}}\right)^{(n)}$,
- (v) $GAH(G) = \left(\frac{2\sqrt{2}}{3}\right)^{(4n+1)} \cdot \left(\frac{\sqrt{3}}{2}\right)^{(9n+1)} \cdot \left(\frac{4}{5}\right)^{(n)} \cdot \left(\frac{2\sqrt{6}}{5}\right)^{(18n-1)} \cdot \left(\frac{4\sqrt{3}}{7}\right)^{(n)}$.

Proof 1. To construct the vertex and edge partitions, we consider the following notations.

$$V_i = \{u \in V(G) : d(u) = i\}, E_i = \{uv \in E(G) : d(u) + d(v) = i\},$$

$$E_i^* = \{uv \in E(G) : d(u)d(v) = i\}.$$

It is clear from the structure analysis of G (Figure 3.1) that $|V(G)| = 49n + 6$, $|E(G)| = 54n + 5$. The vertex and edge partitions of G are shown in Table 4.1, and Table 4.2 respectively.

Figure 3.4: The molecular graph of H_k for $k \geq 1$.

Therefore, using the vertex and edge partitions of $SP[n]$ in the formulation of multiplicative topological indices, we derive the following results.

$$\begin{aligned}
 W_1^s(G) &= \prod_{u \in V(G)} (d(u))^s \\
 &= \prod_{u \in V_1} (d(u))^s \cdot \prod_{u \in V_2} (d(u))^s \cdot \prod_{u \in V_3} (d(u))^s \cdot \prod_{u \in V_4} (d(u))^s \\
 &= 2^{s(18n+4)} \cdot 3^{(20ns)}
 \end{aligned}$$

Figure 3.5: The molecular graph of H_1 , H_2 and H_3 , respectively.Table 4.1: Vertex partition of $SP[n]$.

Partition of $V(G)$	V_1	V_2	V_3	V_4
Frequency	$2(6n + 1)$	$4(4n + 1)$	$20n$	n

$$\begin{aligned}
 MZ_1^a(G) &= \prod_{uv \in E(G)} (d(u) + d(v))^a \\
 &= \prod_{uv \in E_2^*} (d(u) + d(v))^a \cdot \prod_{uv \in E_3^*} (d(u) + d(v))^a \cdot \prod_{uv \in E_4 \cap E_4^*} (d(u) + d(v))^a \\
 &\quad \cdot \prod_{uv \in E_5 \cap E_4^*} (d(u) + d(v))^a \cdot \prod_{uv \in E_5 \cap E_6^*} (d(u) + d(v))^a \cdot \prod_{uv \in E_6 \cap E_8^*} (d(u) + d(v))^a \\
 &\quad \cdot \prod_{uv \in E_6 \cap E_9^*} (d(u) + d(v))^a \cdot \prod_{uv \in E_7 \cap E_{12}^*} (d(u) + d(v))^a \\
 &= [3^a]^{(2n+1)} \cdot [4^a]^{(9n+1)} \cdot [5^a]^{(n)} \cdot [4^a]^{(5n+4)} \cdot [5^a]^{(18n-1)} \cdot [6^a]^{(2n)} \cdot [6^a]^{(16n)} \\
 &\quad \cdot [7^a]^{(n)} \\
 &= 2^{2a(23n+5)} \cdot 3^{a(20n+1)} \cdot 5^{a(19n-1)} \cdot 7^{(an)}.
 \end{aligned}$$

Table 4.2: Edge partition of $SP[n]$.

Partition of $E(G)$	E_2^*	E_3^*	$E_4 \cap E_4^*$	$E_5 \cap E_4^*$	$E_5 \cap E_6^*$
Frequency	$2n + 1$	$9n + 1$	$5n + 4$	n	$18n - 1$
Partition of $E(G)$	$E_6 \cap E_8^*$	$E_6 \cap E_9^*$	$E_7 \cap E_{12}^*$		
Frequency	$2n$	$16n$	n		

$$\begin{aligned}
 MZ_2^a(G) &= \prod_{uv \in E(G)} (d(u)d(v))^a \\
 &= \prod_{uv \in E_2^*} (d(u)d(v))^a \cdot \prod_{uv \in E_3^*} (d(u)d(v))^a \cdot \prod_{uv \in E_4 \cap E_4^*} (d(u)d(v))^a \cdot \\
 &\quad \prod_{uv \in E_5 \cap E_4^*} (d(u)d(v))^a \cdot \prod_{uv \in E_5 \cap E_6^*} (d(u)d(v))^a \cdot \prod_{uv \in E_6 \cap E_8^*} (d(u)d(v))^a \cdot \\
 &\quad \prod_{uv \in E_6 \cap E_9^*} (d(u)d(v))^a \cdot \prod_{uv \in E_7 \cap E_{12}^*} (d(u)d(v))^a \\
 &= [2^a]^{(2n+1)} \cdot [3^a]^{(9n+1)} \cdot [4^a]^{(n)} \cdot [4^a]^{(5n+4)} \cdot [6^a]^{(18n-1)} \cdot [8^a]^{(2n)} \cdot [9^a]^{(16n)} \\
 &\quad \cdot [12^a]^{(n)} \\
 &= 2^{8a(5n+1)} \cdot 3^{(60an)}.
 \end{aligned}$$

$$\begin{aligned}
 ABC(G) &= \prod_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} \\
 &= \left(\frac{1}{\sqrt{2}}\right)^{(2n+1)} \cdot \left(\sqrt{\frac{2}{3}}\right)^{(9n+1)} \cdot \left(\frac{\sqrt{3}}{2}\right)^{(n)} \cdot \left(\frac{1}{\sqrt{2}}\right)^{(5n+4)} \cdot \left(\frac{1}{\sqrt{2}}\right)^{(18n-1)} \\
 &\quad \cdot \left(\frac{1}{\sqrt{2}}\right)^{(2n)} \cdot \left(\frac{2}{3}\right)^{(16n)} \cdot \left(\frac{\sqrt{5}}{2\sqrt{3}}\right)^{(n)} \\
 &= \left(\frac{1}{\sqrt{2}}\right)^{(27n+4)} \cdot \left(\sqrt{\frac{2}{3}}\right)^{(9n+1)} \cdot \left(\frac{\sqrt{3}}{2}\right)^{(n)} \cdot \left(\frac{4}{5}\right)^{(n)} \cdot \left(\frac{2}{3}\right)^{(16n)} \cdot \left(\frac{\sqrt{5}}{2\sqrt{3}}\right)^{(n)}.
 \end{aligned}$$

$$GAH(G) = \prod_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}$$

$$\begin{aligned}
&= \left(\frac{2\sqrt{2}}{3}\right)^{(2n+1)} \cdot \left(\frac{\sqrt{3}}{2}\right)^{(9n+1)} \cdot \left(\frac{4}{5}\right)^{(n)} \cdot (1)^{(5n+4)} \cdot \left(\frac{2\sqrt{6}}{5}\right)^{(18n-1)} \cdot \\
&\quad \left(\frac{2\sqrt{2}}{3}\right)^{(2n)} \cdot (1)^{(16n)} \cdot \left(\frac{4\sqrt{3}}{7}\right)^{(n)} \\
&= \left(\frac{2\sqrt{2}}{3}\right)^{(4n+1)} \cdot \left(\frac{\sqrt{3}}{2}\right)^{(9n+1)} \cdot \left(\frac{4}{5}\right)^{(n)} \cdot \left(\frac{2\sqrt{6}}{5}\right)^{(18n-1)} \cdot \left(\frac{4\sqrt{3}}{7}\right)^{(n)}.
\end{aligned}$$

Hence the proof.

Putting $s = 1, 2, a = 1, 2, -\frac{1}{2}$, in Theorem 1, we obtain the following corollary.

Corollary 1. *Different multiplicative degree based indices of $SP[n]$ are given by,*

- (i) $NK(G) = 2^{2(9n+2)} \cdot 3^{(20n)}$,
- (ii) $\Pi_1(G) = 2^{4(9n+2)} \cdot 3^{(40n)}$,
- (iii) $\Pi_1^*(G) = 2^{2(23n+5)} \cdot 3^{(20n+1)} \cdot 5^{(19n-1)} \cdot 7^{(n)}$,
- (iv) $H\Pi_1(G) = 2^{4(23n+5)} \cdot 3^{2(20n+1)} \cdot 5^{2(19n-1)} \cdot 7^{(2n)}$,
- (v) $SC\Pi(G) = 2^{-(23n+5)} \cdot 3^{-\left(\frac{20n+1}{2}\right)} \cdot 5^{-\left(\frac{19n-1}{2}\right)} \cdot 7^{-\left(\frac{n}{2}\right)}$,
- (vi) $\Pi_2(G) = 2^{8(5n+1)} \cdot 3^{(60n)}$,
- (vii) $H\Pi_2(G) = 2^{16(5n+1)} \cdot 3^{(120n)}$,
- (viii) $PC\Pi(G) = 2^{-4(5n+1)} \cdot 3^{(-30n)}$.

4.2. Multiplicative topological indices of polynomial chain of n -cycles.

The structure of the polynomial chain of n -cycles for $n = 8$ is shown in the Figure 3.2. We construct the vertex and edge partitions of polynomial chain of n -cycles in the following tableau (Table 4.3 and Table 4.4) using the same notations as prescribed in the Theorem 1.

Now, using the vertex (Table 4.3) and edge partitions (Table 4.4) for the polynomial chain of n -cycles in the formulation of multiplicative topological indices, we derive the following results like previous.

Theorem 2. *Let G be the polynomial chain of n -cycles. Then we have*

Table 4.3: Vertex partition of the polynomial chain of n -cycles.

Partition of $V(G)$	V_2	V_3
Frequency	$4(4n + 1)$	$2(4n - 1)$

 Table 4.4: Edge partition of the polynomial chain of n -cycles.

Partition of $E(G)$	$E_4 \cap E_4^*$	$E_5 \cap E_6^*$	$E_6 \cap E_9^*$
Frequency	$4(3n + 1)$	$8n$	$2(4n - 1)$

- (i) $W_1^s(G) = 2^{s(16n+4)} \cdot 3^{s(8n-2)}$,
- (ii) $MZ_1^a(G) = 2^{a(32n+5)} \cdot 3^{a(8n-3)} \cdot 5^{18an}$,
- (iii) $MZ_2^a(G) = 2^{2a(21n+4)} \cdot 3^{2a(17n-3)}$,
- (iv) $ABC(G) = \left(\frac{1}{\sqrt{2}}\right)^{4(5n+1)} \cdot \left(\frac{2}{3}\right)^{(8n-3)}$,
- (v) $GAH(G) = \left(\frac{2\sqrt{6}}{5}\right)^{(8n)}$.

Now putting $s = 1, 2, a = 1, 2, -\frac{1}{2}$, in Theorem 2, we obtain the following corollary.

Corollary 2. *Different multiplicative degree based indices for the polynomial chain of n -cycles are given by,*

- (i) $NK(G) = 2^{4(4n+1)} \cdot 3^{2(4n-1)}$,
- (ii) $\Pi_1(G) = 2^{8(4n+1)} \cdot 3^{4(4n-1)}$,
- (iii) $\Pi_1^*(G) = 2^{(32n+5)} \cdot 3^{(8n-3)} \cdot 5^{(18n)}$,
- (iv) $H\Pi_1(G) = 2^{2(32n+5)} \cdot 3^{2(8n-3)} \cdot 5^{(36n)}$,
- (v) $SC\Pi(G) = 2^{\frac{-32n-5}{2}} \cdot 3^{\left(\frac{-8n+3}{2}\right)} \cdot 5^{-9n}$,
- (vi) $\Pi_2(G) = 2^{2(21n+4)} \cdot 3^{2(17n-3)}$,
- (vii) $H\Pi_2(G) = 2^{4(21n+4)} \cdot 3^{4(17n-3)}$,
- (viii) $PC\Pi(G) = 2^{-(21n+4)} \cdot 3^{-(17n-3)}$.

4.3. Multiplicative topological indices of the triangular benzenoid T_n .

The vertex and edge partitions of the triangular benzenoid T_n are shown in Table 4.5 and Table 4.6, respectively.

Table 4.5: Vertex partition of the triangular benzenoid T_n .

Partition of $V(G)$	V_2	V_3
Frequency	$3(n+1)$	n^2+n-2

Table 4.6: Edge partition of the triangular benzenoid T_n .

Partition of $E(G)$	$E_4 \cap E_4^*$	$E_5 \cap E_6^*$	$E_6 \cap E_9^*$
Frequency	6	$\frac{3n(n-1)}{2}$	$6(n-1)$

Therefore, using the vertex and edge partitions for the triangular benzenoid T_n in the formulation of multiplicative topological indices, we derive the following results.

Theorem 3. *Let G be the triangular benzenoid T_n . Then we have*

- (i) $W_1^s(G) = 2^{s(3n+3)} \cdot 3^{s(n^2+n-2)},$
- (ii) $MZ_1^a(G) = 2^{6a(n+1)} \cdot 3^{6a(n-1)} \cdot 5^{\frac{3an(n-1)}{2}},$
- (iii) $MZ_2^a(G) = 2^{\frac{3a(n^2-n+8)}{2}} \cdot 3^{\frac{3a(n+8)(n-1)}{2}},$
- (iv) $ABC(G) = (\frac{1}{\sqrt{2}})^{3(n^2-n+4)} \cdot (\frac{2}{3})^{6(n-1)},$
- (v) $GAH(G) = (\frac{2\sqrt{6}}{5})^{\frac{3n(n-1)}{2}}.$

Now putting $s = 1, 2, a = 1, 2, -\frac{1}{2}$, in Theorem 3, we obtain the following corollary.

Corollary 3. *Different multiplicative degree based indices for the polynomial chain of n -cycles are given by,*

- (i) $NK(G) = 2^{3(n+1)} \cdot 3^{(n^2+n-2)}$,
- (ii) $\Pi_1(G) = 2^{6(n+1)} \cdot 3^{2(n^2+n-2)}$,
- (iii) $\Pi_1^*(G) = 2^{6(n+1)} \cdot 3^{6(n-1)} \cdot 5^{\frac{3n(n-1)}{2}}$,
- (iv) $H\Pi_1(G) = 2^{12(n+1)} \cdot 3^{12(n-1)} \cdot 5^{3n(n-1)}$,
- (v) $SC\Pi(G) = 2^{-3(n+1)} \cdot 3^{-3(n-1)} \cdot 5^{\frac{-3n(n-1)}{4}}$,
- (vi) $\Pi_2(G) = 2^{\frac{3(n^2-n+8)}{2}} \cdot 3^{\frac{3(n+8)(n-1)}{2}}$,
- (vii) $H\Pi_2(G) = 2^{3(n^2-n+8)} \cdot 3^{3(n+8)(n-1)}$,
- (viii) $PC\Pi(G) = 2^{\frac{-3(n^2-n+8)}{4}} \cdot 3^{\frac{-3(n+8)(n-1)}{4}}$.

4.4. Multiplicative topological indices of the circumcoronene series of benzenoid (H_k , $k \geq 1$).

Finally, we aim to determine the multiplicative degree based indices for circumcoronene series of benzenoid. Its vertex and edge partitions are shown in Table 4.7 and Table 4.8, respectively.

Table 4.7: Vertex partition of the circumcoronene series of benzenoid H_k .

Partition of $V(G)$	V_2	V_3
Frequency	$6k$	$6k(k-1)$

Table 4.8: Edge partition of the circumcoronene series of benzenoid H_k .

Partition of $E(G)$	$E_4 \cap E_4^*$	$E_5 \cap E_6^*$	$E_6 \cap E_9^*$
Frequency	6	$12(k-1)$	$9k^2 - 15k + 6$

Thus, using the vertex and edge partitions for the circumcoronene series of benzenoid (H_k) in the formulation of multiplicative topological indices, we obtain the following theorem as before.

Theorem 4. Let G be the circumcoronene series of benzenoid (H_k). Then we have

- (i) $W_1^s(G) = 2^{(6ks)} \cdot 3^{6ks(k-1)},$
- (ii) $MZ_1^a(G) = 2^{3a(3k^2-5k+6)} \cdot 3^{3a(3k^2-5k+2)} \cdot 5^{12a(k-1)},$
- (iii) $MZ_2^a(G) = 2^{(12ak)} \cdot 3^{18ak(k-1)},$
- (iv) $ABC(G) = 2^{3(3k^2-7k+3)} \cdot 3^{-3(3k^2-5k+2)},$
- (v) $GAH(G) = \left(\frac{2\sqrt{6}}{5}\right)^{12(k-1)}.$

Now putting $s = 1, 2, a = 1, 2, -\frac{1}{2}$, in Theorem 4, we obtain the following corollary.

Corollary 4. Different multiplicative degree based indices for the circumcoronene series of benzenoid (H_k) are given by,

- (i) $NK(G) = 2^{(6k)} \cdot 3^{6k(k-1)},$
- (ii) $\Pi_1(G) = 2^{(12k)} \cdot 3^{12k(k-1)},$
- (iii) $\Pi_1^*(G) = 2^{3(3k^2-5k+6)} \cdot 3^{3(3k^2-5k+2)} \cdot 5^{12(k-1)},$
- (iv) $H\Pi_1(G) = 2^{6(3k^2-5k+6)} \cdot 3^{6(3k^2-5k+2)} \cdot 5^{24(k-1)},$
- (v) $SC\Pi(G) = 2^{\frac{-3(3k^2-5k+6)}{2}} \cdot 3^{\frac{-3(3k^2-5k+2)}{2}} \cdot 5^{-6(k-1)},$
- (vi) $\Pi_2(G) = 2^{(12k)} \cdot 3^{18k(k-1)},$
- (vii) $H\Pi_2(G) = 2^{(24k)} \cdot 3^{36k(k-1)},$
- (viii) $PC\Pi(G) = 2^{(-6k)} \cdot 3^{-9k(k-1)}.$

Conclusion

Because of the controversial evolution of viruses, many new diseases can be discovered every year. That is why, new drug design is required to treat new diseases. Topological index play vital role to design novel drug as per diseases. In this work, we have put some efforts to obtain some multiplicative degree based topological indices of certain molecular graphs that widely appear in drug structures. Further, the results are plotted

Figure 4.1: Plotting of topological indices against their parameters. By $\log(TI)$, we mean the logarithm of topological indices.

against their parameters in Figure 4.1. These theoretical results might be helpful to understand the underlying topology of the aforesaid chemical structures. As a future work, we would like to continue this work for some nanostar dendrimers.

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