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TOPOLOGICAL INDICES OF DISCRETE MOLECULAR STRUCTURE

Muhammad Aamer Rashid*, Sarfraz Ahmad

Department of Mathematics, COMSATS University Islamabad, Lahore Campus, 54000, Pakistan

Juan L.G. Guirao

Technical University of Cartagena, Department of Applied Mathematics and Statistics
Hospital de Marina, 30203-Cartagena, SPAIN

Najma Abdul Rehman and Muhammad Kamran Siddiqui

Department of Mathematics, COMSATS University Islamabad, Sahiwal Campus, 57000, Pakistan

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Abstract. Topological indices defined on molecular structures can help researchers better understand the physical features, chemical reactivity, and biological activity. Thus, the study of the topological indices on chemical structure of chemical materials and drugs can make up for lack of chemical experiments and can provide a theoretical basis for the manufacturing of drugs and chemical materials. In this paper, we focus on the family of smart polymer which is widely used in anticancer drugs manufacturing. In chemical graph theory, a topological index is a numerical representation of a chemical structure which correlates certain physico-chemical characteristics of underlying chemical compounds e.g., boiling point and melting point). More preciously, we focus on the family of smart polymer which is widely used in anticancer drugs manufacturing, and computed exact results for degree based topological indices.

1. **Introduction.** Chemical Graph theory is playing an important role among the most uncommon and unique branch of science by which the appearing of any structure is made conceivable. Starting late, it accomplishes much thought among researchers because of its broad assortment of uses in Computer science, electrical frameworks, interconnected frameworks, natural systems, and in science, et cetera. It helps in understanding about the essential properties of an atomic diagram. There are an impressive measure of atomic mixes, which have collection of uses in the fields of pharmaceutical science, consistently life and anticancer drugs.
In this era of rapid technological development, chemical and pharmaceutical techniques in recent years have been rapidly evolved, and thus a large number of new nanomaterials, crystalline materials, and drugs emerge every year. To determine the chemical properties of such a large number of new compounds and new drugs requires a large amount of chemical experiments, thereby greatly increasing the workload of the chemical and pharmaceutical researchers. Fortunately, the chemical based experiments found that there was strong connection between topology

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* Corresponding author: Muhammad Aamer Rashid.

molecular structures and their physical behaviors, chemical characteristics, and biological features, such as melting point, boiling point, and toxicity of drugs (see Wiener [1] and Katritzky et al. [2]).
Another subject specifically Chem-informatics which is a mix of chemistry, arithmetic and data science serves to examines $(QSAR)$ and $(QSPR)$ associations that are utilized to foresee the bioactivity and physiochemical properties of chemical compounds. A topological index is a numerical regard that is handled scientifically from the molecular graph. It is connected with compound constitution exhibiting for relationship of substance structure with various physical, and natural activities [3, 4, 5].
For a given $G = (V, E)$ diagram where V to be the vertex set and E to be the edge set of G. The degree $\xi(r)$ of r is the amount of edges of G episode with r. The length of a most restricted way in a diagram G is a separation $d(r, s)$ among r and s. A graph can be spoken by a polynomial, a numerical esteem or by network shape. There are certain sorts of topological indices principally degree based idices and distances based indices.
In 1972, Gutman and Trinajestic [6, 7] define the Zagreb indices as:

$$M_1(G) = \sum_{rs \in E(G)} (\zeta(r) + \zeta(s)) \tag{1}$$

$$M_2(G) = \sum_{uv \in E(G)} (\zeta(r) \cdot \zeta(s)) \tag{2}$$

In 2008, Došlić itroduces the first and second Zagreb coindex as: [8]:

$$\overline{M_1} = \overline{M_1}(G) = \sum_{rs \notin E(G)} [\zeta(r) + \zeta(s)] \tag{3}$$

$$\overline{M_2} = \overline{M_2}(G) = \sum_{rs \notin E(G)} \zeta(r)\zeta(s) \tag{4}$$

In 2016, I. Gutman *et al.* [9] proves the following Theorems:

Theorem 1.1. *Let G be a graph with $|V(G)|$ vertices and $|E(G)|$ edges and $M_1(G)$ represent the first zagreb index, then*

$$\overline{M_1}(G) = 2|E(G)|\Big(|V(G) - 1\Big) - M_1(G) \tag{5}$$

Theorem 1.2. *Let G be a graph with $|V(G)|$ vertices and $|E(G)|$ edges and $M_1(G)$, $M_2(G)$ represent the first and second zagreb index respectively, then*

$$\overline{M_2}(G) = 2|E(G)|^2 - \frac{1}{2}M_1(G) - M_2(G) \tag{6}$$

B. Furtula and I. Gutman [12] introduced forgotten topological index (also called F-index) as:

$$F(G) = \sum_{rs \in E(G)} \left(\zeta(r)^2 + \zeta(s)^2\right) \tag{7}$$

Some latest result regarding forgotten topological index see [13]
Spurred by the achievement of the ABC index, Furtula [14] *et.al.*, set forth its changed adaptation and they named it "Augmented Zagreb index" and is characterized as:

$$AZI(G) = \sum_{rs \in E(G)} \left(\frac{\zeta(r)\zeta(s)}{\zeta(r) + \zeta(s) - 2} \right)^3 \tag{8}$$

Another topological index in view of the level of the vertex is the Balaban index [15, 16]. This index for a graph G of order n, size m is characterized as:

$$J(G) = \frac{m}{m - n + 2} \sum_{rs \in E(G)} \frac{1}{\sqrt{\zeta(r) \times \zeta(s)}} \tag{9}$$

In 2009, Furtula et al. [6] introduced Atom-Bond Connectivity (ABC) index, which it has been applied up until now to study the stability of alkanes and the strain energy of cyclo alkanes. This index is defined as follows

$$ABC(G) = \sum_{uv \in EG} \sqrt{\frac{\zeta(r) + \zeta(s) - 2}{\zeta(r) \times \zeta(s)}} \tag{10}$$

Although several advances have been made in PI index, Zagreb index, Wiener index, hyper-Wiener index, and sum connectivity index of different kinds of molecular graphs, the study of topological indices for Dox-loaded micelle comprising PEG-PAsp block copolymer with chemically conjugated Dox has been largely limited. In addition, this kind of smart polymer structures is widely used in medical science and pharmaceutical field. For example, it plays a key role in delivery system and in the development of anticancer drugs. Based on these reasons, industrial interest and tremendous academic interest have been attracted to research the topological indices of this molecular structure from a mathematical point of view see [18, 19, 20, 21, 22, 23].
In the following contents, we first introduce the smart polymers of Dox-loaded micelle comprising PEG-PAsp block copolymer with chemically conjugated Dox and explain the importance of this molecular structure. This is the reason why we focus on the topological indices computation on this family of molecular graphs. Then in next Section , we present our main results and detailed proofs.

2. **Methods.** For the calculation of our outcomes, we used a methodology for combinatorial enlisting, a vertex segment procedure, an edge parcel procedure, diagram theoretical instruments, logical frameworks, a degree-tallying technique, and a degrees of neighbors system. Also, we utilized Matlab for logical estimations and affirmations. We moreover used Maple for plotting numerical outcomes.

3. **Literature Review and Motivation.** As a special class of macromolecules, smart polymers manifest impressive response to physio chemical change if their circumstance has slight interference, for example, changes on PH value, ionic disturbance, magnetic field, light, and temperature (see Hai and Broek mann [24], do Nascimento Marques et al. [25], and Kroning et al. [26]. Thus, smart polymers are also denoted by environmentally responsive systems or stimuli responsive ones. As good delivery systems, these structures have wide applications in biomedical field, for instance, smart polymers with nucleic acid or protein delivery to intracellular targets just like nucleus or ribosome in tissue engineering (see Chonkar et al. [27], Hrub'Y et al. [28], Duro-Castano et al. [29], and Khandare and Calder' on [30]. As

a special class of smart polymer, polymeric micelles (e.g., Dox-conjugated PEG-b-poly(aspartate) (PEG-PAsp) block copolymers; see Shanthi et al. [31] and Osada et al. [32] are widely applied in delivering anticancer drug.

4. **Molecular Structure of SP[n].** The Dox-loaded micelle containing PEG-PAsp block copolymer with chemically conjugated Dox (see Figure 1 for its detailed structure) is a famous family of smart polymer which is used as anthracycline anticancer antibiotic and applied in treating various kinds of cancers. It is employed as excipient and drug delivery carriers for strengthening the stability and the times of drug retention.Thus, it has powerful anticancer activity and is widely considered in the pharmacy field (see Nishiyama and Kataoka [33] and Butt et al. [34] for more details). As can be seen in Figure 1, the integer number n is step of growth in this kind of polymers. We depict the structure of Dox-loaded micelle containing PEG-PAsp block copolymer with chemically conjugated Dox when n=1,2 and 3 (see figures 1(b), 2(a) and 2(b) resp.)

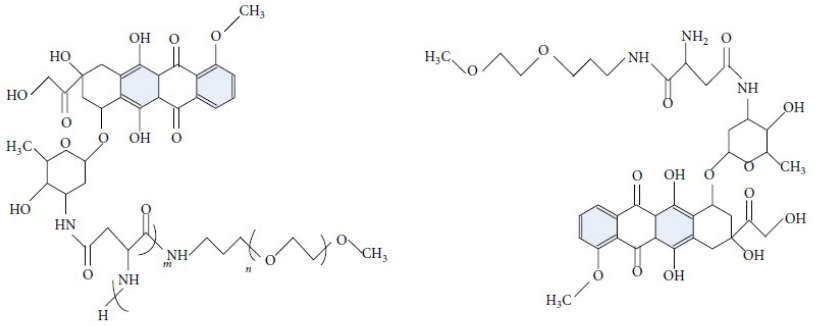

FIGURE 1. (a) SP[n] (b) SP[1]

4.1. **Results for Molecular Structure of SP[n].** The number of vertices and edges in $SP[n]$ are $49n+6$ and $54n+5$ respectively. Now first we compute degree based topological indices for $SP[n]$. There are eight types of edge partitions based on the end degrees for each vertex.
The first edge partition contains $2n+1$ edges rs, where $\zeta(r)=1$ and $\zeta(s)=2$. The second edge partition contains $9n+1$ edges rs, where $\zeta(r)=1$ and $\zeta(s)=3$. The third edge partition contains n edges rs, where $\zeta(r)=1$ and $\zeta(s)=4$. The fourth edge partition contains $5n+4$ edges rs, where $\zeta(r)=2$ and $\zeta(s)=2$. The fifth edge partition contains $18n-1$ edge rs, where $\zeta(r)=2$ and $\zeta(s)=3$. The sixth edge partition contains $2n$ edges rs, where $\zeta(r)=2$ and $\zeta(s)=4$. The seventh edge partition contains $16n$ edges rs, where $\zeta(r)=3$ and $\zeta(s)=3$. The eighth edge partition contains n edge rs, where $\zeta(r)=3$ and $\zeta(s)=4$.

- **The first and second zagreb indices of** $SP[n]$

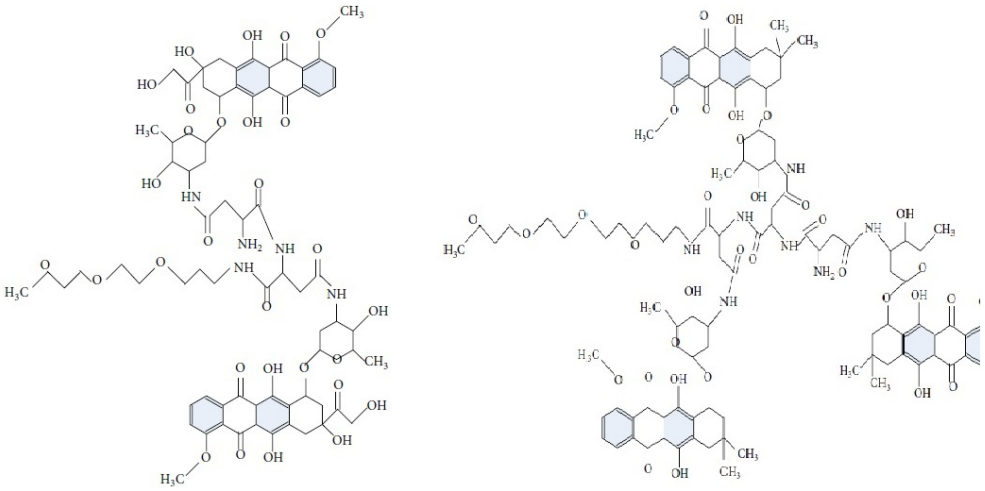

FIGURE 2. (a) SP[2] (b) SP[3]

$$\begin{aligned} M_1(SP[n]) &= 272n + 8 \\ M_2(SP[n]) &= 335n + 15 \end{aligned}$$

- **The first and second zagreb coindices of** $SP[n]$

Now by using Equations (5) and Theorem 1 first Zagreb coindex is computed as below:

$$\begin{aligned} \overline{M_1}(G) &= \sum_{rs \notin E(G)} (\zeta(r) + \zeta(s)) \\ \overline{M_1}(G) &= 2|E(G)|\big(|V(G)| - 1\big) - M_1(G) \\ &= 2(54n + 5)\big(49n + 6 - 1\big) - (272n + 8) \\ &= 5292n^2 + 758n + 32 \end{aligned}$$

Now, by using Equations (6) and Theorem 2, the second zagreb coindex is computed as:

$$\begin{aligned} \overline{M_2}(G) &= \sum_{rs \notin E(G)} (\zeta(r)\zeta(s)) \\ &= 2|E(G)|^2 - \frac{1}{2}M_1(G) - M_2(G) \\ \overline{M_2}(G) &= 2(54n + 5)^2 - \frac{1}{2}(272n + 8) - (335n + 15) \\ &= 5832n^2 + 609n + 26 \end{aligned}$$

- **Forgotten index, Augmented zagreb index, Balaban index and ABC index of SP[n]**

Let G be the graph of $SP[n]$. Then by using Equation (7), the forgotten index is computed as:

$$\begin{aligned} F(G) &= \sum_{rs\in E(G)} \left(\zeta(r)^2+\zeta(s)^2\right) \\ &= (1^2+2^2)(2n+1)+(1^2+3^2)(9n+1)+(1^2+4^2)(12)+(2^2+2^2)(n) \\ &+ (2^2+3^2)(18n-1)+(2^2+4^2)(2n)+(3^2+3^2)(16n)+(3^2+4^2)(n) \\ &+ (2^2+3^2)(5n+4) \\ &= 744n+34 \end{aligned}$$

Now by using Equation (8), the augmented zagreb index is computed as:

$$\begin{aligned} AZI(G) &= \sum_{rs\in E(G)} \left(\frac{\zeta(r)\zeta(s)}{\zeta(r)+\zeta(s)-2}\right)^3 \\ &= \left(\frac{1*2}{1+2-2}\right)^3(6)+\left(\frac{1*3}{1+3-2}\right)^3(12(n-1)) \\ &+ \left(\frac{2*2}{2+2-2}\right)^3(6(n-2))+\left(\frac{2*3}{2+3-2}\right)^3(6(n-1)) \\ &+ \left(\frac{3*3}{3+3-2}\right)^3(12(n-2))+\left(\frac{3*4}{3+4-2}\right)^3(9n^2-21n+12) \\ &+ \left(\frac{1*4}{1+4-2}\right)^3(12)+\left(\frac{2*4}{2+4-2}\right)^3(12) \\ &= \frac{976729}{2250}n+\frac{137}{4} \end{aligned}$$

Now by using Equations (9), Balaban index is computed as below:

$$\begin{aligned} J(G) &= \frac{m}{m-n+2}\sum_{rs\in E(G)}\frac{1}{\sqrt{\zeta(r)\times\zeta(s)}} \\ &= \frac{54n+5}{54n+5-49n-6+2}\Big[\frac{2n+1}{\sqrt{1\times2}}+\frac{9n+1}{\sqrt{1\times3}}+\frac{n}{\sqrt{1\times4}} \\ &+\frac{5n+4}{\sqrt{2\times2}}+\frac{18n-1}{\sqrt{2\times3}}+\frac{2n}{\sqrt{2\times4}}+\frac{16n}{\sqrt{3\times3}}+\frac{n}{\sqrt{3\times4}}\Big] \end{aligned}$$

Now by using Equations (10), ABC index is computed as below:

$$\begin{aligned} ABC(G) &= \sum_{rs\in E(G)} \sqrt{\frac{\zeta(r)+\zeta(s)-2}{\zeta(r)\times\zeta(s)}} \\ &= \sqrt{\frac{1+2-2}{1\times 2}}(2n+1)+\sqrt{\frac{1+3-2}{1\times 3}}(9n+1)+\sqrt{\frac{1+4-2}{1\times 4}}(n) \\ &+ \sqrt{\frac{2+3-2}{2\times 3}}(18n-1)+\sqrt{\frac{2+4-2}{2\times 4}}(2n)+\sqrt{\frac{3+3-2}{3\times 3}}(16n) \\ &+ \sqrt{\frac{2+2-2}{2\times 2}}(5n+4)+\sqrt{\frac{3+4-2}{3\times 4}}(n) \\ &= \sqrt{\frac{1}{2}}(2n+1)+\sqrt{\frac{2}{3}}(9n+1)+\sqrt{\frac{3}{4}}(n)+\sqrt{\frac{1}{2}}(5n+4) \\ &+ \sqrt{\frac{1}{2}}(18n-1)+\sqrt{\frac{1}{2}}(2n)+\sqrt{\frac{4}{9}}(16n)+\sqrt{\frac{5}{12}}n \end{aligned}$$

5. **Comparisons and Discussion.**

- For the comparison of these indices numerically for $SP[n]$, we computed all indices for different values of n. Now, from Table 1 we can easily see that all indices are in increasing order as the values of n are increasing. The graphical representations of the topological indices for $SP[n]$ are depicted in Figure 3(a) and 3(b), for certain values of n.

TABLE 1. Numerical computation of all indices for $SP[n]$.

n	$\overline{M_1(G)}$	$\overline{M_2(G)}$	$F(G)$	$AZI(G)$	$J(G)$,	$ABC(G)$
1	6082	6467	778	468.4	257.2	42.27
2	22716	24572	1522	902.5	507.9	80.87
3	49934	54341	2266	1337	759.1	119.5
4	87736	95776	3010	1771	1010	158.2

- The forgotten topological index is helpful for testing the substance and pharmacological properties of drug nuclear structures. So in the case of $SP[n]$, its increasing value is useful for quick action during chemical reaction for drugs. The augmented Zagreb index displays a good correlation with the formation heat of heptanes and octane. So our computation for $AZI(G)$ index is play an important rule for formation heat of heptane and octane as its values are in increasing order.

6. **Conclusion.** In this paper, we have studied and computed some degree based topological indices for $SP[n]$. The exact results have been computed of first and second Zegreb coindices, forgotten index, the augmented Zagreb index, Balaban index, and $ABC(G)$ index of $SP[n]$. Also we provide the numerically and graphically representation of these indices. As these result are help in chemical point of you as

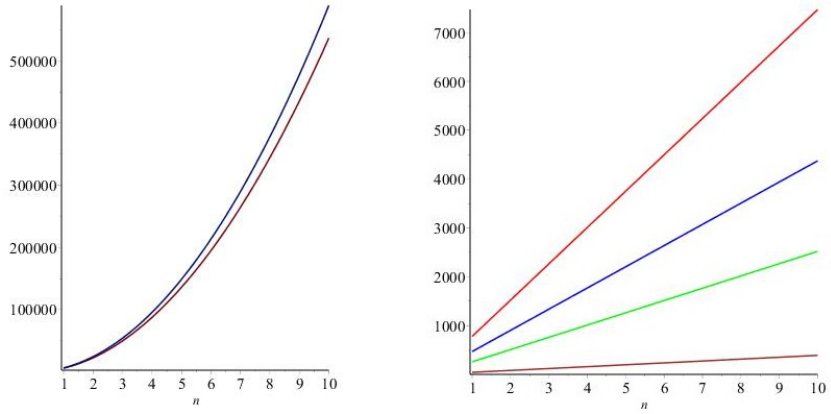

FIGURE 3. (a) $\overline{M_1(G)}(red)$, $\overline{M_2(G)}(blue)$, (b) F(G)(red), AZI(G)(blue), J(G)(green), ABC(G)(brown)

well as pharmaceutical science, we are looking forward in future to compute other topological indices for $SP[n]$.

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E-mail address: aamerrasheed7869@gmail.com
E-mail address: sarfrazahmad@cuilahore.edu.pk
E-mail address: juan.garcia@upct.es
E-mail address: $najma_$ar@hotmail.com
E-mail address: kamransiddiqui75@gmail.com