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Novel Distance-Based Molecular Descriptors for Styrene Butadiene Rubber Structures

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ABSTRACT

Styrene-butadiene rubber (SBR) is a general-purpose rubber produced from a copolymer of styrene and butadiene. It is used largely in automobile and truck tires. In general, it is considered to be an abrasion-resistant replacement for natural rubber. In this article, we compute a set of recently introduced distance-based topological descriptors namely, Zagreb connection indices and reformulated Zagreb connection indices for the SBR structures. Zagreb indices and Reformulated Zagreb indices were applied to forecast numerous molecular properties through QSAR studies of boiling point, Molar volume and bioactivity. These indices offer a quick and effective measure of molecular complexity and features of their composition resulting in approximate molecular behavior.

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A. INTRODUCTION

Chemical Graph Theory is one of the significant branches of graph theory that plays a vital role in addressing several real-time problems in the field of Mathematical Chemistry. A molecular graph, or chemical graph, is an important tool to analyze the properties or characteristics of chemical compounds (Randić, M., 2008). It plays a significant role in drug design. In a molecular graph, each vertex represents an atom, and every edge represents the bond between any two atoms of a chemical compound. The topological index is one of the best tools in mathematical chemistry which helps chemists in performing QSAR/QSPR studies of a chemical compound. It is actually a numerical value associated with each molecular graph, and it is also a graph invariant. In general, there are two major types of topological indices: degree-

based indices and distance-based indices. Degree-based indices such as Zagreb indices, Randić index, Harary index, and Harmonic index are well-studied graph parameters. Similarly, the Wiener index is one of the oldest distance-based topological indices. In recent years, some new distance-based indices have been introduced and studied by researchers. To name a few, the Mostar index, and the leap Zagreb indices. The leap Zagreb indices or the Zagreb connection indices are distance-based topological indices introduced in 2017 and further expend in (Manjunatha et al., 2020). The first, second and third Zagreb connection indices are defined as follows:

$$ZC_1(G) = \sum_{v \in V(G)} \tau(v)^2 \tag{1}$$

$$ZC_2(G) = \sum_{uv \in E(G)} \tau(u)\tau(v) \tag{2}$$

$$ZC_3(G) = \sum_{v \in V(G)} \deg(v)\tau(v) \tag{3}$$

where $\tau(v)$ denotes the connection number of a vertex v in a graph G, that is the number of vertices which are of distance two from v in G. Also, Ali et al. (2022) studied the first leap Zagreb index of some graph operations. Similarly, one can find the results on the third leap Zagreb index of some graph operations in (Liu et al., 2020a). Further, Chidambaram et al. (2020) studied the properties of leap graphs, which are based on the second degree of a vertex of a graph. Ghalavand et al. (2022) studied the Zagreb connection indices of some nanostructures. In this article, he renamed the leap Zagreb indices as Zagreb Connection Indices. Since then, researchers have been using both terminologies in their articles. In the present article, we use the terminology of Zagreb connection indices for leap Zagreb indices. Liu et al. (2020a) obtained some new results on the Zagreb connection indices of disjunction and symmetric difference operations on graphs. Ali et al. (2020) discussed the modified Zagreb connection indices of the T-sum graphs. Alsinai et al. (2022) introduced the concept of reciprocal leap indices of graphs and studied their properties. Asif et al. (2020) studied some leap indices of polycyclic aromatic hydrocarbons. Furthermore, Asif et al. (n.d.) discussed computational results on some special types of networks known as -networks via the Zagreb connection indices. Cao et al. (2020) discussed the Zagreb connection indices of molecular graphs based on some operations. Dehgardi et al. (2021) found bounds on the first leap Zagreb index of trees. Dehgardi & Aram (2021) studied the Zagreb connection indices of two dendrimer stars. Gutman et al. (2020) investigated leap-Zagreb indices of trees and unicyclic graphs. Liu et al. (2020b) computed Zagreb connection numbers for cellular neural networks. Manjunatha et al. (2020) introduced and studied the properties of a new set of disatance-degree based descriptors called leap Zagreb indices (also known as Zagreb connection indices). Further Chidambaram et al. (2020) investigated the first leap Zagreb indices of some graph operations. Manjunatha et al. (2020) studied some properties of leap graphs. Also, Ghalavand et al. (2023) studied the second leap Zagreb index of some graph

operations. Raza et al. (2023) studied the leap Zagreb connection index for some network models. Chidambaram et al. (2020) obtained some results on the leap Zagreb indices of bridge and chain graphs. Raza et al. (2023) computed Zagreb connection indices for some benzenoid systems. Liu et al. (2020b) investigated the Zagreb connection indices of hex and honeycomb networks. Homepage et al. (2021) computed Connection-Based Multiplicative Zagreb Indices of Dendrimer Nanostars Also, Ashraful Alam et al. (2022); Salamat et al. (2021) computed connection based topological indices of dendrimers. For more details on other topological invariants, one may refer to (Delen et al., 2022; Kamran et al., 2023). Motivated by the definitions of Zagreb connection indices(also called Leap Zagreb indices) given in Dehgardi et al. (2021), recently, Natarajan et al. have introduced a new set of distance-based topological indices namely, reformulated Zagreb connection indices and studied them for anti-viral drugs used in the treatment of COVID-19 pandemic. The definitions of the three reformulated Zagreb connection indices are given below:

$$RZC_1(G) = \sum_{e \in E(G)} \tau(e)^2 \tag{4}$$

where $\tau(e) = \tau(u) + \tau(v) - 2$ for an edge $e = uv$ in G.

$$RZC_2(G) = \sum_{e \sim f} \tau(e)\tau(f) \tag{5}$$

where $e \sim f$ denote a pair of adjacent edges in G.

$$RZC_3(G) = \sum_{e \in EG)} \deg(e)\tau(e) \tag{6}$$

where $\deg(e) = \deg(u) + \deg(v) - 2$ for an edge $e = uv$ in G.

Styrene-butadiene rubber (SBR) is a general-purpose rubber produced from a copolymer of styrene and butadiene. It is used largely in automobile and truck tires. In general, it is considered an abrasion-resistant replacement for natural rubber. Butadiene and styrene are combined to form SBR, which is 75% Butadiene and 25% Styrene. Most recently, Kamran et al. (2022) studied M-polynomials and some degree-based topological indices for SBR structures. This research work provides the motivation for us to compute the Zagreb connection indices and the reformulated Zagreb connection indices for SBR structures. Figures 1 - 3 show the structure of SBR Polymers.

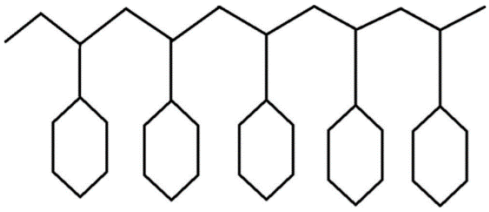

Figure 1. SBR – Type A ($\mathfrak{R}_1$)

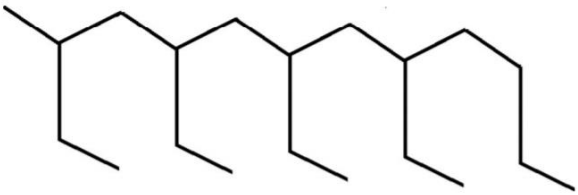

Figure 2. SBR – Type B ($\mathfrak{R}_2$)

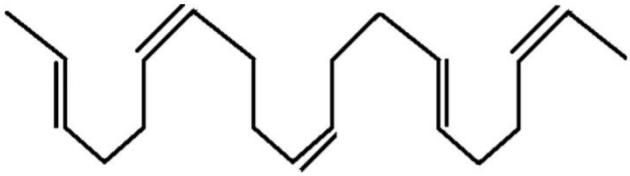

Figure 3. SBR – Type C ($\mathfrak{R}_3$)

B. MATERIALS AND METHODS

We use the vertex partition and the edge partition methods to obtain partition tables (Tables 1-18). These tables are mainly used to compute the proposed topological indices for the graphs that represent SBR structures. When considering SBR structures to study, it is important to employ the vertex partition and edge partition as the two primary methods to sort and study the connectivity offered by molecular graphs. Vertex partition refers to the process of grouping the vertices or atoms of the graph into subsets or partitions based on a specific criterion. The same is true for the edge partition, where subsets of edges or bonds are created based on additional characteristics. sing these partitioning techniques, we produced partition tables (Tables 1–18) that offer a methodical breakdown of the edges and vertices of the SBR structures in accordance with the partitions to which they belong. These tables provide an extensive summary of the structural makeup of the molecular graphs and are useful reference materials.

C. RESULT AND DISCUSSION

Note that in the following Theorems, denotes the usual multiplication. The computation of Zagreb connection indices of SBR discussed from one end also requires a deep understanding of the meaning and implications of these indices in the analysis of molecular graphs, as well as their importance in chemistry and other domains. Indeed, Zagreb indices describe the structural patterns of molecules and provide far-reaching insights into their chemistry and reactivity. In case of SBR structures, their computation reveals connectivity patterns in simplified molecules, thus exposing certain patterns concerning their behavior and potential applications in various domains, including drug design and materials science. In addition, this

work emphasized (usual multiplication) in the context of each of these theorems deliberated underscores the mathematics aspect of these computational processes, which makes the results more rigorous and applicable in various disciplines.

1. Computation of Zagreb Connection Indices of SBR Structures

In this section, we compute the three Zagreb coneection indices (also known an leap Zagreb indices) for the three SBR structures namely, $\mathfrak{R}_1, \mathfrak{R}_2$ and $\mathfrak{R}_3$. The vertex and edge partition tables are given in Tables 1-9.

Table 1. Connection number based vertex partition of $\mathfrak{R}_1$

Vertex v with $\tau(v)$)	**1**	**2**	**3**	**4**
Frequency	1	$3n+2$	$2n+1$	$3n-2$

Table 2. Connection number based edge partition of $\mathfrak{R}_1$

Edge uv with $(\tau(u), \tau(v))$	$(1,2)$	$(2,2)$	$(2,3)$	$(2,4)$	$(3,4)$	$(4,4)$
Frequency	1	$2n$	$2n+1$	1	$2n+2$	$3n-4$

Table 3. Degree and connection number based vertex partition of $\mathfrak{R}_1$

Vertex v with $(\boldsymbol{deg}(v), \boldsymbol{\tau}(v))$	$(1,1)$	$(1,2)$	$(2,2)$	$(2,3)$	$(2,4)$	$(3,3)$	$(3,4)$
Frequency	1	1	$3n+1$	$2n$	$n-1$	1	$2n-1$

Theorem 1

i. $ZC_1(\mathfrak{R}_1) = 78n - 14$
ii. $ZC_2(\mathfrak{R}_1) = 92n - 24$
iii. $ZC_3(\mathfrak{R}_1) = 56n - 4$

Proof:

(i) From the vertex partition given in Table-1, we have

$$\begin{aligned} ZC_1(\mathfrak{R}_1) &= \sum_{v \in V(\mathfrak{R}_1)} (\tau(v))^2 \\ &= 1^2(1) + 2^2(3n+2) + 3^2(2n+1) + 4^2(3n-2) \\ &= 1 + 12n + 8 + 18n + 9 + 48n - 32 \end{aligned} \tag{7}$$

Therefore,

$$\mathrm{ZC}_1(\mathfrak{R}_1) = 78n - 14. \tag{8}$$

(ii) Using the edge partition given in Table-2, we get

$$ZC_2(\Re_1) = \sum_{uv \in E(\Re_1)} \tau(u)\tau(v)$$
$$= (1*2)(1) + (2*2)(2n) + (2*3)(2n+1) + (2*4)(1) + (3*4)(2n+2) + (4*4)(3n-4) \quad (9)$$
$$= 2 + 8n + 6(2n+1) + 8 + 12(2n+2) + 16(3n-4)$$
$$= 2 + 8n + 12n + 6 + 8 + 24n + 24 + 48n - 64$$

Therefore,

$$\mathrm{ZC}_2(\Re_1) = 92n - 24. \quad (10)$$

(ii) From the vertex partition given in Table-3, we have

$$ZC_3(\Re_1) = \sum_{v \in V(\Re_1)} \deg(v)\tau(v)$$
$$= (1*1)(1) + (1*2)(1) + (2*2)(3n+1) + (2*3)(2n) + (2*4)(n-1) + (3*3)(1) + (3*4)(2n-1) \quad (11)$$
$$= 1 + 2 + 4(3n+1) + 6(2n) + 8(n-1) + 9 + 12(2n-1)$$
$$= 1 + 2 + 12n + 4 + 12n + 8n - 8 + 9 + 24n - 12$$

Thus,

$$ZC_3(\Re_1) = 56n - 4. \quad (12)$$

Table 4. Connection number based vertex partition of $\Re_2$

$\boldsymbol{\tau(v)}$	**1**	**2**	**3**	**4**
Frequency	$n+1$	$n+2$	$n-1$	$n-2$

Table 5. Connection number based edge partition of $\Re_2$

$(\boldsymbol{\tau(u), \tau(v)})$	$(\mathbf{1,1})$	$(\mathbf{1,2})$	$(\mathbf{2,2})$	$(\mathbf{2,3})$	$(\mathbf{2,4})$	$(\mathbf{3,3})$	$(\mathbf{3,4})$
Frequency	1	n	2	$n-1$	1	1	$2n-5$

Table 6. Degree and connection number based vertex partition of $\Re_2$

$(\boldsymbol{deg, \tau(v)})$	$(\mathbf{1,1})$	$(\mathbf{1,2})$	$(\mathbf{2,2})$	$(\mathbf{2,3})$	$(\mathbf{2,4})$	$(\mathbf{3,3})$
Frequency	n	2	n	2	$n-2$	$n-2$

Theorem 2

i. $ZC_1(\Re_2) = 30n - 32$

ii. $ZC_2(\Re_2) = 32n - 40$

iii. $ZC_3(\Re_2) = 22n - 18$

Proof:

(i) From the vertex partition given in Table 4, we have

$$ZC_1(\mathfrak{R}_2) = \sum_{v \in V(\mathfrak{R}_2)} \tau(v)^2$$
$$= 1^2(n+1) + 2^2(n+2) + 3^2(n-1) + 4^2(n-2)$$
$$= 1(n+1) + 4(n+2) + 9(n-1) + 16(n-2) \quad (13)$$
$$= n + 1 + 4n + 8 + 9n - 9 + 16n - 32$$

Therefore,

$$ZC_1(\mathfrak{R}_2) = 30n - 32. \quad (14)$$

(ii) By virtue of the edge partition given in Table 5, we get

$$ZC_2(\mathfrak{R}_2) = \sum_{uv \in E(\mathfrak{R}_2)} \tau(u)\tau(v)$$
$$= (1*1)(1) + (1*2)(n) + (2*2)(2) + (2*3)(n-1)$$
$$+(2*4)(1) + (3*3)(1) + (3*4)(2n-5) \quad (15)$$
$$= 1 + 2n + 8 + 6(n-1) + 8 + 9 + 12(2n-5)$$
$$= 1 + 2n + 8 + 6n - 6 + 8 + 9 + 24n - 60$$

Hence,

$$ZC_2(\mathfrak{R}_2) = 32n - 40. \quad (16)$$

(ii) Using the vertex partition given in Table 6, we have

$$ZC_3(\mathfrak{R}_2) = \sum_{v \in V(\mathfrak{R}_2)} \deg(v)\tau(v)$$
$$= (1*1)(n) + (1*2)(2) + (2*2)(n) + (2*3)(2)$$
$$+(2*4)(n-2) + (3*3)(n-2) + \quad (17)$$
$$= n + 4 + 4n + 12 + 8(n-2) + 9(n-2)$$
$$= n + 4 + 4n + 12 + 8n - 16 + 9n - 18$$

Therefore,

$$ZC_3(\mathfrak{R}_2) = 22n - 18. \quad (18)$$

Table 7. Connection number based vertex partition of $\mathfrak{R}_3$

Vertex v with $\tau(v)$	**1**	**2**
Frequency	4	4n-4

Table 8. Connection number based edge partition of $\mathfrak{R}_3$

Edge uv with $(\tau(u), \tau(v))$	$(1,1)$	$(1,2)$	$(2,2)$
Frequency	2	2	$4n-5$

Table 9. Degree and connection number based vertex partition of $\mathfrak{R}_3$

Vertex v with $(deg(v), \tau(v))$	$(1,1)$	$(1,2)$	$(2,2)$
Frequency	2	2	$4n-4$

Theorem 3

i. $ZC_1(\mathfrak{R}_3) = 16n - 12$

ii. $ZC_2(\mathfrak{R}_3) = 16n - 14$

iii. $ZC_3(\mathfrak{R}_3) = 16n - 10$

Proof:

(i) With the help of Table 7, we get

$$\begin{aligned} ZC_1(\mathfrak{R}_3) &= \sum_{v \in V(\mathfrak{R}_3)} \tau(v)^2 \\ &= 1^2(4) + 2^2(4n-4) \\ &= 4 + 4(4n-4) \\ &= 4 + 16n - 16 \end{aligned} \tag{19}$$

Therefore,

$$ZC_1(\mathfrak{R}_3) = 16n - 12. \tag{20}$$

From Table 8, we have

$$\begin{aligned} ZC_2(\mathfrak{R}_3) &= \sum_{uv \in E(\mathfrak{R}_3)} \tau(u)\tau(v) \\ &= (1*1)(2) + (1*2)(2) + (2*2)(4n-5) \\ &= 2 + 4 + 4(4n-5) \\ &= 2 + 4 + 16n - 20 \end{aligned} \tag{21}$$

Thus, we get

$$ZC_2(\mathfrak{R}_3) = 16n - 14. \tag{22}$$

(ii) Using Table 9 we get,

$$\begin{aligned} ZC_3(\mathfrak{R}_3) &= \sum_{v \in V(\mathfrak{R}_3)} \deg(v)\tau(v) \\ &= (1*1)(2) + (1*2)(2) + (2*2)(4n-4) \\ &= 2 + 4 + 4(4n-4) \\ &= 2 + 4 + 16n - 16 \end{aligned} \tag{23}$$

Therefore,

$$ZC_3(\mathfrak{R}_3) = 16n - 10. \tag{24}$$

2. Computation of Reformulated Zagreb Connection Indices of $\mathfrak{R}_1, \mathfrak{R}_2$ *and* $\mathfrak{R}_3$

Table 10. Connection number based edge partition of $\mathfrak{R}_1$

Edge e with $\boldsymbol{\tau(e)}$	**1**	**2**	**3**	**4**	**5**	**6**
Frequency	1	$2n$	$2n+1$	1	$2n+2$	$3n-4$

Table 11. Connection number based edge partition of $\mathfrak{R}_1$

Edges $\boldsymbol{e \sim f}$ **with** $(\boldsymbol{\tau(e), \tau(f)})$	$(\mathbf{1,4})$	$(\mathbf{2,2})$	$(\mathbf{2,3})$	$(\mathbf{3,5})$	$(\mathbf{4,6})$	$(\mathbf{5,5})$	$(\mathbf{5,6})$	$(\mathbf{6,6})$
Frequency	1	n	$2n$	$2n+2$	2	$n+3$	$2n-1$	$4n-7$

Table 12. Degree and connection number based edge partition of $\mathfrak{R}_1$

Edge e with $(\boldsymbol{deg(e), \tau(e)})$	(1,1)	(2,2)	(2,3)	(3,4)	(3,5)	(3,6)	(4,5)	(4,6)
Frequency	1	$2n$	$2n+1$	1	$2n+1$	$2n-3$	1	$n-1$

Theorem 4

i. $RZC_1(\mathfrak{R}_1) = 184n - 68$

ii. $RZC_2(\mathfrak{R}_1) = 275n - 125$

iii. $RZC_3(\mathfrak{R}_1) = 110n - 24$

Proof:

(i) From the edge partition given in Table 10, we have

$$\begin{aligned} RZC_1(\mathfrak{R}_1) &= \sum_{e \in E(\mathfrak{R}_1)} \tau(e)^2 \\ &= 1^2(1) + 2^2(2n) + 3^2(2n+1) + 4^2(1) + 5^2(2n+2) \\ &\quad + 6^2(3n-4) \\ &= 1 + 4(2n) + 9(2n+1) + 16 + 25(2n+2) + 36(3n-4) \\ &= 1 + 8n + 18n + 9 + 16 + 50n + 50 + 108n - 144 \end{aligned} \tag{25}$$

Thus,

$$\mathrm{RZC}_1(\mathfrak{R}_1) = 184n - 68. \tag{26}$$

(ii) Using the edge partition given in Table 11, we get

$$RZC_2(\Re_1) = \sum_{e\sim f} \tau(e)\tau(f)$$
$$= (1*4)(1) + (2*2)(n) + (2*3)(2n) + (3*5)(2n+2) + (4*6)(2) + (5*5)(n+3) + (5*6)(2n-1) + (6*6)(4n-7)$$
$$= 4 + 4n + 12n + 15(2n+2) + 24(2) + 25(n+3) + 30(2n-1) + 36(4n-7)$$
$$= 4 + 4n + 12n + 30n + 30 + 48 + 25n + 75 + 60n - 30 + 144n - 252 \quad (27)$$

Therefore,

$$RZC_2(\Re_1) = 275n - 125. \quad (28)$$

(iii) With the help of the edge partition in Table 12, we have

$$RZC_3(\Re_1) = \sum_{e\in E(\Re_1)} \deg(e)\tau(e)$$
$$= (1*1)(1) + (2*2)(2n) + (2*3)(2n+1) + (3*4)(1) + (3*5)(2n+1) + (3*6)(2n-3) + (4*5)(1) + (4*6)(n-1)$$
$$= 1 + 4(2n) + 6(2n+1) + 12 + 36n - 54 + 30n + 15 + 24n - 24 + 20$$
$$= 1 + 8n + 12n + 6 + 12 + 36n - 54 + 30n + 15 + 24n - 21 + 20 \quad (29)$$

Therefore,

$$RZC_3(\Re_1) = 110n - 24. \quad (30)$$

Table 13. Connection number based edge partition of $\Re_2$

$\boldsymbol{\tau(e)}$	**0**	**1**	**2**	**3**	**4**	**5**
Frequency	1	n-1	2	$n-1$	2	$2n-5$

Table 14. Connection number based adjacent edge partition of $\Re_2$

$(\boldsymbol{\tau(e)}, \boldsymbol{\tau(f)})$	(0,1)	(1,2)	(1,3)	(2,2)	(3,5)	(4,5)
Frequency	1	1	$n-1$	1	$2n-5$	2

Table 15. Degree and Connection number based edge partition of $\Re_2$

$(\boldsymbol{deg(e)}, \boldsymbol{\tau(e)})$	$(\mathbf{0},\mathbf{1})$	$(\mathbf{1},\mathbf{1})$	$(\mathbf{1},\mathbf{2})$	$(\mathbf{2},\mathbf{2})$	$(\mathbf{2},\mathbf{3})$	$(\mathbf{3},\mathbf{3})$	$(\mathbf{3},\mathbf{4})$	$(\mathbf{3},\mathbf{5})$
Frequency	1	$n-1$	1	1	2	$n-2$	2	$2n-5$

Theorem 5

i. $RZC_1(\Re_2) = 60n - 95$
ii. $RZC_2(\Re_2) = 33n - 32$
iii. $RZC_3(\Re_2) = 40n - 52$

Proof:

(i)

$$RZC_1(\Re_2) = \sum_{e \in E(\Re_2)} \tau(e)^2$$

$$\begin{aligned} &= 0^2(1) + 1^2\,(\text{n-1}) + 2^2(2) + 3^2(n-1) + 4^2(2) \\ &\quad + 5^2(2n-5) \\ &= 0 + n - 1 + 4(2) + 9(-1) + 16(2) + 25(2n-5) \\ &= n - 1 + 8 + 9n - 9 + 32 + 50n - 125 \end{aligned} \tag{31}$$

$$\mathrm{RZC}_1(\Re_2) = 60n - 95$$

(ii)

$$RZC_2(\Re_2) = \sum_{e \sim f} \tau(e)\tau(f)$$

$$\begin{aligned} &= (0*1)(1) + (1*2)(1) + (1*3)(n-1) + (2*2)(1) \\ &\quad + (3*5)(2n-5) + (4*5)(2) \\ &= 0 + 2 + 3(n-1) + 4 + 15(2n-5) + 20(2) \\ &= 2 + 3n - 3 + 4 + 30n - 75 + 40 \end{aligned} \tag{32}$$

$$RZC_2(\Re_2) = 33n - 32$$

(iii)

$$RZC_3(\Re_2) = \sum_{e \in E(\Re_2)} \deg(e)\tau(e)$$

$$\begin{aligned} &= (0*1)(1)(1*1)(n-1) + (1*2)(1) + (2*2)(1) \\ &\quad + (2*3)(2) + (3*3)(n-2) + (3*4)(2) \\ &\quad + (3*5)(2n-5) \\ &= n - 1 + 2 + 4 + 12 + 9(n-2) + 24 + 15(2n-5) \\ &= n - 1 + 2 + 4 + 12 + 9n - 18 + 24 + 30n - 75 \end{aligned} \tag{33}$$

$$RZC_3(\Re_2) = 40n - 52$$

Table 16. Connection number based edge partition of $\Re_3$

$\boldsymbol{\tau(e)}$	**Frequency**
0	2
1	2
2	$4n-5$

Table 17. Connection number based adjacent edges partition of $\Re_3$

$\boldsymbol{e \sim f}$ **with** $(\boldsymbol{\tau(e), \tau(f)})$	(0,1)	(1,2)	(1,3)
Frequency	2	2	$4n-6$

Table 18. Degree and connection number based edge partition of $\Re_3$

$(\boldsymbol{deg(e), \tau(e)})$	(0,1)	(1,1)	(1,2)
Frequency	2	2	$4n-5$

Theorem 6

i. $RZC_1(\mathfrak{R}_3) = 16n - 18$

ii. $RZC_2(\mathfrak{R}_3) = 16n - 20$

iii. $RZC_3(\mathfrak{R}_3) = 16n - 16$

Proof:

(i) By virtue of Table 16 , we have

$$\begin{aligned} RZC_3(\mathfrak{R}_2) &= \sum_{e \in E(\mathfrak{R}_2)} \deg(e)\tau(e) \\ RZC_1(\mathfrak{R}_3) &= \sum_{e \in E(\mathfrak{R}_3)} \tau(e)^2 \\ &= 0^2(2) + 1^2(2) + 2^2(4n-5) \\ &= 2 + 4(4n-5) \\ &= 2 + 16n - 20 \end{aligned} \tag{34}$$

Therefore,

$$\mathrm{RZC}_1(\mathfrak{R}_3) = 16n - 18. \tag{35}$$

(ii) From Table 17, we get

$$\begin{aligned} RZC_2(\mathfrak{R}_3) &= \sum_{e \sim f} \tau(e)\tau(f) \\ &= (0*1)(2) + (1*2) + (2*2)(4n-6) \\ &= 4 + 4(4n-6) \\ &= 4 + 16n - 24 \end{aligned} \tag{36}$$

Thus, we have

$$RZC_2(\mathfrak{R}_3) = 16n - 20. \tag{37}$$

(ii) From Table 18, we have

$$\begin{aligned} RZC_3(\mathfrak{R}_3) &= \sum_{e \in E(\mathfrak{R}_3)} \deg(e)\tau(e) \\ &= (0*1)(1) + (2*1)(2) + (2*2)(4n-5) \\ &= 4 + 4(4n-5) \\ &= 4 + 16n - 20 \end{aligned} \tag{38}$$

Thus,

$$RZC_3(\mathfrak{R}_3) = 16n - 16. \tag{39}$$

D. CONCLUSIONS

Topological descriptors are widely used to analyze the physio-chemical properties of drugs and other chemical compounds. In this article, we computed a new set of reformulated Zagreb connection indices, which are the variants of the well-studied Zagreb connection indices for three types of SBR structures. We believe that these results definitely help chemists analyze the properties of SBR structures and derive better results.

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