

## On Comparing Rhombus Oxide and Silicate Networks via Zagreb Connection Indices

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**Abstract.** A topological index (TI) is a number that describes the topology of a chemical structure. TIs can describe numerous chemical and physical properties of chemical compounds, such as melting and freezing points, strain energy, stability, temperature, volume, density, and pressure. TIs are classified into several categories, including degree-based TIs, distance-based TIs, and connection number-based TIs. Wiener developed the first distance-based TI. After that, he developed the first degree-based TI for calculating the  $\pi$ -electron energy of molecules. These indices are regarded as the most important TIs for preserving the psychochemical features of chemical compounds. Recently, connection number-based TIs have been researched, which are more efficient than distance and degree-based TIs. Connection-based TIs can predict the physical and chemical properties of molecular structures more efficiently than degree or distance-based descriptors. In this paper, we compute the connection number-based TIs for the two most significant types of chemical structures: rhombus silicate and rhombus oxide. In the end, to evaluate the effectiveness of these structures in predicting psycho-chemical attributes, we compare them based on their computed results. These findings are novel and make significant contributions to providing knowledge to understand the deep topology of these critical structures.

**AMS (MOS) Subject Classification Codes:** 05C0; 05C92

**Key Words:** Topological Index, Rhomus Silicate, Rhombus Oxide, Molecular Structure, Zagreb Connection Index.

### 1. INTRODUCTION

Cheminformatics represents an emerging interdisciplinary field that melds disciplines namely, information science, mathematics, and chemistry. Within the domain of chemistry, graph theory has found widespread utility. Specifically, chemical graph theory, a subfield of mathematical chemistry, employs graph theory to quantitatively describe chemical phenomena. Over recent decades, extensive research endeavors have been dedicated to this area, culminating in a profound influence on the broader landscape of chemical sciences.

Central to this discipline are topological indices (TIs), numerical values linked to chemical structures, which purport to elucidate associations between a compound's structure and various physico-chemical properties, chemical reactivity, or even biological activity. At its core, the foundation of topological indices rests on the transformation of a molecular graph into a numerical representation that encapsulates the graph's topology. Our investigation delves into unraveling the intricate relationships between a chemical compound's structural attributes, its characteristics, and its bioactivity through molecular modeling. Molecular descriptors play a pivotal role in essential domains such as chemistry and pharmacology. It is worth noting that topological indices have emerged as critical tools in solving QSAR and QSPR [20]. A number, a polynomial, a series of integers, or a matrix that represents the entire graph can be used to identify a graph, and each of these representations aims to be specifically defined for that graph. A topological index is a numerical value that describes the topology of a graph and is unaffected by graph automorphism. Topological indices (TIs) have a vast span of applicability in various other fields of science. They are helpful in predicting the chemical properties of molecular chemical structures such as freezing point, boiling point, volume, density, stability, and strain energy. TIs can be divided into several broad categories, including degree-based TIs, distance-based TIs, polynomial-based TIs, and connection number (CN) based TIs. Among these categories, CN-based TIs are of tremendous significance and are particularly important in chemical graph theory and chemistry.

Wiener [21] developed the first distance-based TI in 1947 to investigate the boiling point of paraffin. Furthermore, Gutman and Trinajstić [9] proposed the first degree-based TI to test the total  $\pi$ -electron energy of an alternative hydrocarbon in 1972. Gutman et al. [8] investigated the concept of second-degree-based TI in 1975. Furtula and Gutman [7] pioneered the concept of the third ZI. Nikolic [15] later introduced the concept of modified first ZI in 2003. Dhanalakshmi et al. [5] proposed the concept of multiplicative ZI. These traditional ZI have been widely used in the field of cheminformatics [1, 4].

Nowadays, the researchers are working on CN-based TIs. A CN is a count of the vertices that are two distances apart from a given vertex. Instead of degree-based ZIs, Zagreb connection indices (ZCI) have a wider range of applicability in determining the physical and chemical properties of chemical substances. According to scientists, ZCIs provide a better platform for measuring chemical attributes such as melting and freezing points, strain energy, stability, temperature, volume, density, and pressure of molecular chemical structures than other classical ZIs. After the development of ZCIs, researchers started utilizing these indices in comprehending the properties of molecular structures. Sattar et al. [16, 17, 18] worked on computing the ZCIs of different chemical structures. Ali and Trinajstić, [3] initiated ZCIs and investigated their applicability on octane isomers. Fatima et al. [6] computed ZCIs of some chemical structures. In addition, Ali et al. [2] discovered modified CN-based ZIs of T-sum graphs. Javaid et al. [11] developed CN-based ZIs for various wheel graphs. For more results, readers are referred to [22, 23, 24]. Javaid and Sattar [12] calculated ZCIs of metal-organic frameworks. For more details about rhombus oxide and silicate [19, 13, 14].

In this research article, we compute the first, second, and third ZCI. Further, we compute modified first, second, and third ZCI, FZCI, modified SZCI, and modified third ZCI of two significant types of chemical structures, namely, rhombus oxide (RHOX) and rhombus silicate (RHSL) network. This manuscript is structured as; section 2 of this research article includes some basic definitions and formulas that are used to compute the main results. Section 3 summarizes the main findings for the rhombus silicate network. We compute the ZCIs for the rhombus oxide network in section 4. Section 5 presents a comparison of the computed TIs of RHSL and RHOX networks and between these networks and covers the concluding remarks. List of Acronyms used in this paper is given in Table 1.

TABLE 1. List of Acronyms

Name	Acronyms
Zagreb connection index	<i>ZCI</i>
Topological index	<i>TI</i>
Connection numbers	<i>CN</i>
First Zagreb Connection Index	<i>FZCI</i>
Second Zagreb Connection Index	<i>SZCI</i>
Third Zagreb Connection Index	<i>SZCI</i>

## 2. NOTATIONS AND PRELIMINARIES

Here, we present some important basic definitions which help to understand the concept of this article. Let  $P = (\mathcal{H}(P), \mathcal{L}(P))$  be a graph, where  $\mathcal{H}(P)$  be the vertex set and  $\mathcal{L}(P)$  be the edge set. The first Zagreb index (FZI) defined in [9] is given by

$$\widehat{\mathcal{Z}}_1(P) = \sum_{h \in \mathcal{H}(P)} (deg_P(h))^2.$$

We can also rewrite the above equation as

$$\widehat{\mathcal{Z}}_1(P) = \sum_{hf \in \mathcal{L}(P)} (deg_P(h) + deg_P(f)),$$

where  $deg_P(h)$  and  $deg_P(f)$  represents the degree of the vertex  $h$  and  $f$ , respectively.

The second Zagreb index (SZI) defined by Gutman and Rusic [8] is given below

$$\widehat{\mathcal{Z}}_2(P) = \sum_{hf \in \mathcal{L}(P)} (deg_P(h) \times deg_P(f)),$$

where  $deg_P(h)$  and  $deg_P(f)$  represent the degree of the vertex  $h$  and  $f$ , respectively.

The first Zagreb connection index (FZCI) and second Zagreb connection index (SZCI) defined by Ali and Trinajstić [3] can be defined as

$$\widehat{\mathcal{Z}}\mathcal{C}_1(P) = \sum_{h \in \mathcal{H}(P)} (\varpi_P(h))^2, \quad (2.1)$$

$$\widehat{\mathcal{Z}}\mathcal{C}_2(P) = \sum_{hf \in \mathcal{L}(P)} (\varpi_P(h) \times \varpi_P(f)), \quad (2.2)$$

where  $\varpi_P(h)$  and  $\varpi_P(f)$  indicate the connection number (CN) of the vertex  $h$  and  $f$ , respectively.

For a graph  $P$ , the modified ZCIs is given below

$$\widehat{\mathcal{ZC}}^*_1(P) = \sum_{hf \in \mathcal{L}(P)} (\varpi_P(h) + \varpi_P(f)) = \sum_{h \in \mathcal{H}(P)} (\widehat{\mathbf{deg}}_P(h) \varpi_P(h)), \quad (2.3)$$

$$\widehat{\mathcal{ZC}}^*_2(P) = \sum_{hf \in \mathcal{L}(P)} [deg_P(h) \varpi_P(f) + deg_P(f) \varpi_P(h)], \quad (2.4)$$

$$\widehat{\mathcal{ZC}}^*_3(P) = \sum_{hf \in \mathcal{L}(P)} [deg_P(h) \varpi_P(h) + deg_P(f) \varpi_P(f)]. \quad (2.5)$$

These modified ZCIs, proposed by Ali [3] and Ali et al. [2], are known as the modified FZCI, modified SZCI and modified TZCI respectively.

Now, we look at how to create RHSL and RHOX networks in this part. By far, the most exciting mineral class is silicate. Metal carbonates and metal oxides are fused with sand to form these networks. All silicates contain the  $SiO_4$  tetrahedron as a fundamental unit. In chemistry, the vertices in the corners of the  $SiO_4$  tetrahedron represent oxygen ions, whereas the vertices in the middle represent silicon ions. In graph theory, the corner vertices are termed oxygen nodes, whereas the center vertices are termed silicon nodes. By assembling the tetrahedron silicate in various ways, new silicate structures may be created. Similarly, diverse silicate structures create unique silicate networks. Figure 3, depicts the RHSL network of dimension 3, i.e.,  $RHSL(3)$ . By deleting the silicon ions from the RHSL network, we obtained the RHOX network as depicted in Figure 6. In the present study, we denote the RHSL and RHOX networks of dimension  $s$  by  $RHSL(s)$  and  $RHOX(s)$ . In general, the total count of vertices and edges in  $RHSL(s)$  are  $5s^2 + 2s$  and  $12s^2$ , respectively. Further, the total count of vertices and edges in  $RHOX(s)$  network are  $3s^2 + 2s$  and  $6s^2$ , respectively. Now, we move towards the main results of this paper.

### 3. ZCIs OF RHSL NETWORK

In this section, we calculate the ZCIs for RHSL networks. Let  $P = RHSL(s)$ , be a molecular graph RHSL network, where  $s \geq 2$  is the dimension of the network. In Figure 1, Figure 2 and Figure 3, we represent the molecular graph of  $P = (\mathcal{H}, \mathcal{L})$  of  $RHSL(s)$  for  $s = 2, 3, 4$  by labeling the vertices with the their CNs. For this, let us define the partitions of the vertices which are based on the CNs of the vertices. From Figure 3, we can see that there are six vertex-based partitions as given below.

$$\begin{aligned} \mathcal{H}_5 &= \{h \in \mathcal{H}(P) : \varpi(h) = 5\}, \\ \mathcal{H}_6 &= \{h \in \mathcal{H}(P) : \varpi(h) = 6\}, \\ \mathcal{H}_9 &= \{h \in \mathcal{H}(P) : \varpi(h) = 9\}, \\ \mathcal{H}_{12} &= \{h \in \mathcal{H}(P) : \varpi(h) = 12\}, \\ \mathcal{H}_{15} &= \{h \in \mathcal{H}(P) : \varpi(h) = 15\}, \\ \mathcal{H}_{18} &= \{h \in \mathcal{H}(P) : \varpi(h) = 18\}, \end{aligned}$$

The total number of vertices in each partitions are given in Table 2. Adding all the vertices of each partition gives the total number of vertices of  $RHSL(s)$  network. Similarly, we define the edge partitions. From Figure 3, we can see that there are thirteen edge-based partitions as given below.

$$\begin{aligned} \mathcal{L}_{(5,5)} &= \{hf \in \mathcal{L}(P) : \varpi(h) = 5, \varpi(f) = 5\}, \\ \mathcal{L}_{(5,6)} &= \{hf \in \mathcal{L}(P) : \varpi(h) = 5, \varpi(f) = 6\} \\ \mathcal{L}_{(5,12)} &= \{hf \in \mathcal{L}(P) : \varpi(h) = 5, \varpi(f) = 12\} \end{aligned}$$

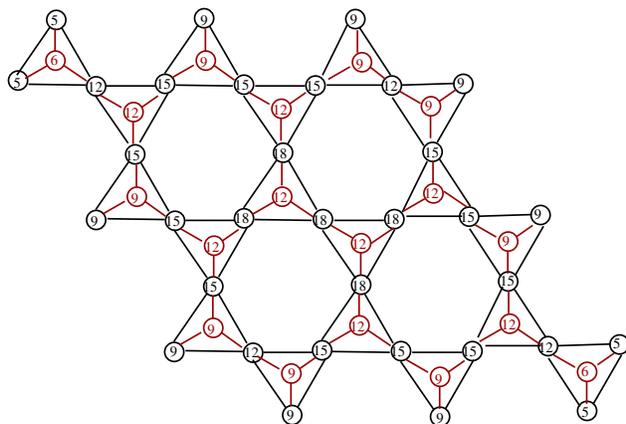


FIGURE 1. RHSL(3) along with the CN each vertex.

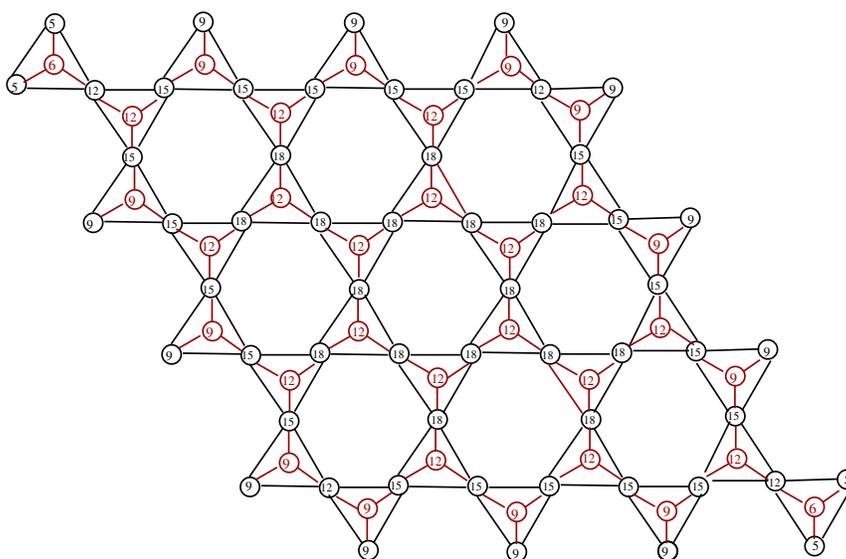


FIGURE 2. RHSL(4) along with the CN each vertex

$$\mathcal{L}_{(6,12)} = \{hf \in \mathcal{L}(P) : \varpi(h) = 6, \varpi(f) = 12\},$$

$$\mathcal{L}_{(9,9)} = \{hf \in \mathcal{L}(P) : \varpi(h) = 9, \varpi(f) = 9\},$$

$$\mathcal{L}_{(9,12)} = \{hf \in \mathcal{L}(P) : \varpi(h) = 9, \varpi(f) = 12\},$$

$$\mathcal{L}_{(9,15)} = \{hf \in \mathcal{L}(P) : \varpi(h) = 9, \varpi(f) = 15\},$$

$$\mathcal{L}_{(12,12)} = \{hf \in \mathcal{L}(P) : \varpi(h) = 12, \varpi(f) = 12\},$$

$$\mathcal{L}_{(12,15)} = \{hf \in \mathcal{L}(P) : \varpi(h) = 12, \varpi(f) = 15\},$$

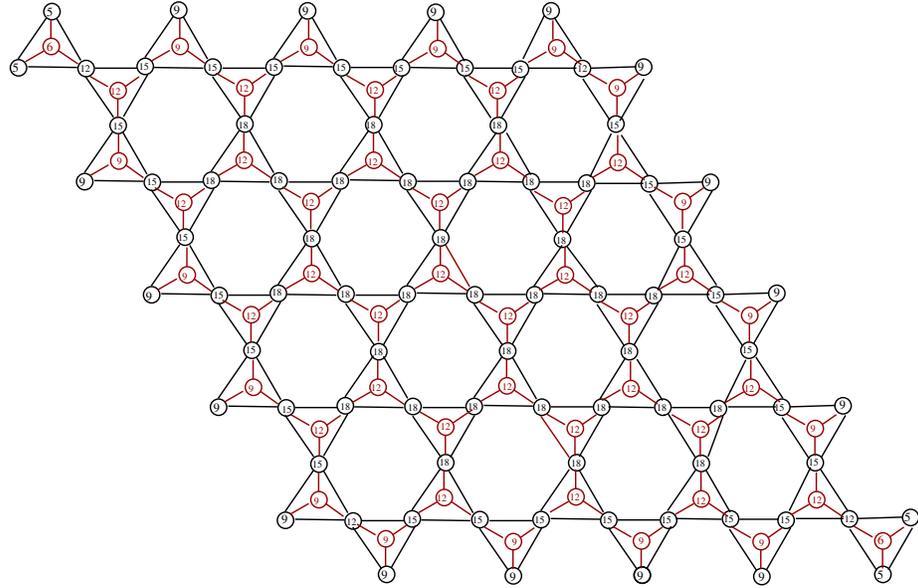


FIGURE 3. RHSL(5) along with the CN each vertex

TABLE 2. Total number of vertices in each partition

$\mathcal{H}_{\varpi(h)}$	$ \mathcal{H}_{\varpi(h)} $
$\mathcal{H}_5$	4
$\mathcal{H}_6$	2
$\mathcal{H}_9$	$8s - 8$
$\mathcal{H}_{12}$	$2s^2 - 4s + 6$
$\mathcal{H}_{15}$	$8s - 12$
$\mathcal{H}_{18}$	$3s^2 - 10s + 8$

$$\mathcal{L}_{(12,18)} = \{hf \in \mathcal{L}(P) : \varpi(h) = 12, \varpi(f) = 18\},$$

$$\mathcal{L}_{(15,15)} = \{hf \in \mathcal{L}(P) : \varpi(h) = 15, \varpi(f) = 15\},$$

$$\mathcal{L}_{(15,18)} = \{hf \in \mathcal{L}(P) : \varpi(h) = 15, \varpi(f) = 18\},$$

$$\mathcal{L}_{(18,18)} = \{hf \in \mathcal{L}(P) : \varpi(h) = 18, \varpi(f) = 18\}.$$

The cardinalities of above partitioned edge are given in Table 3.

**Theorem 3.1.** Let  $P$  be a molecular graph of RHSL network. Then FZCI is given by

$$\widehat{\mathcal{Z}}\mathcal{C}_1(P) = 1260s^2 - 1368s + 280.$$

TABLE 3. Count of CN-based classified edges of  $P$ 

$\mathcal{L}_{(h,f)}$	$ \mathcal{L}_{(h,f)} $
$\mathcal{L}_{(5,5)}$	2
$\mathcal{L}_{(5,6)}$	4
$\mathcal{L}_{(5,12)}$	4
$\mathcal{L}_{(6,12)}$	2
$\mathcal{L}_{(9,9)}$	$4s - 4$
$\mathcal{L}_{(9,12)}$	8
$\mathcal{L}_{(9,15)}$	$16s - 24$
$\mathcal{L}_{(12,12)}$	2
$\mathcal{L}_{(12,15)}$	$8s - 4$
$\mathcal{L}_{(12,18)}$	$6s^2 - 20s + 16$
$\mathcal{L}_{(15,15)}$	$8s - 14$
$\mathcal{L}_{(15,18)}$	$8s - 16$
$\mathcal{L}_{(18,18)}$	$6s^2 - 24s + 24$

**Proof:** By using Table 2 and Equation 2.1, we get

$$\begin{aligned}
\widehat{\mathcal{Z}}\mathcal{C}_1(P) &= \sum_{h \in \mathcal{H}(P)} (\varpi_P(h))^2, \\
&= |\mathcal{H}_5|(\varpi_P(h))^2 + |\mathcal{H}_6|(\varpi_P(h))^2 + |\mathcal{H}_9|(\varpi_P(h))^2 \\
&\quad + |\mathcal{H}_{12}|(\varpi_P(h))^2 + |\mathcal{H}_{15}|(\varpi_P(h))^2 + |\mathcal{H}_{18}|(\varpi_P(h))^2, \\
&= 4(5)^2 + 2(6)^2 + (8s - 8)(9)^2 + (2s^2 - 4s + 6)(12)^2 \\
&\quad + (8s - 12)(15)^2 + (3s^2 - 10s + 8)(18)^2, \\
&= 172 + (648s - 648) + (288s^2 - 576s + 864) + (1800s - 2700) \\
&\quad + (972s^2 - 3240s + 2592), \\
&= 1260s^2 - 1368s + 280.
\end{aligned}$$

**Theorem 3.2.** Let  $P$  be a molecular graph of RHSL network. Then SZCI is given by

$$\widehat{\mathcal{Z}}\mathcal{C}_2(P) = 3240s^2 - 4212s + 1184.$$

**Proof:** By using Table 3 and Equation 2.2, we get

$$\begin{aligned}
\widehat{\mathcal{Z}}\mathcal{C}_2(P) &= \sum_{hf \in \mathcal{L}(P)} (\varpi_P(h) \times \varpi_P(f)), \\
&= |\mathcal{L}_{(5,5)}|(\varpi_P(h) \times \varpi_P(f)) + |\mathcal{L}_{(5,6)}|(\varpi_P(h) \times \varpi_P(f)) + |\mathcal{L}_{(5,12)}|(\varpi_P(h) \times \varpi_P(f)) \\
&+ |\mathcal{L}_{(6,12)}|(\varpi_P(h) \times \varpi_P(f)) + |\mathcal{L}_{(9,9)}|(\varpi_P(h) \times \varpi_P(f)) + |\mathcal{L}_{(9,12)}|(\varpi_P(h) \times \varpi_P(f)) \\
&+ |\mathcal{L}_{(9,15)}|(\varpi_P(h) \times \varpi_P(f)) + |\mathcal{L}_{(12,12)}|(\varpi_P(h) \times \varpi_P(f)) + |\mathcal{L}_{(12,15)}|(\varpi_P(h) \times \varpi_P(f)) \\
&+ |\mathcal{L}_{(12,18)}|(\varpi_P(h) \times \varpi_P(f)) + |\mathcal{L}_{(15,15)}|(\varpi_P(h) \times \varpi_P(f)) + |\mathcal{L}_{(15,18)}|(\varpi_P(h) \times \varpi_P(f)) \\
&+ |\mathcal{L}_{(18,18)}|(\varpi_P(h) \times \varpi_P(f)), \\
&= 2(5 \times 5) + 4(5 \times 6) + 4(5 \times 12) + 2(6 \times 12) + (4s - 4)(9 \times 9) \\
&+ 8(9 \times 12) + (16s - 24)(9 \times 15) + 2(12 \times 12) + (8s - 4)(12 \times 15) \\
&+ (6s^2 - 20s + 16)(12 \times 18) + (8s - 14)(15 \times 15) + (8s - 16)(15 \times 18) \\
&+ (6s^2 - 24s + 24)(18 \times 18), \\
&= 2(25) + 4(30) + 4(60) + 2(72) + (4s - 4)(81) + 8(108) \\
&+ (16s - 24)(135) + 2(144) + (8s - 4)(180) + (6s^2 - 20s + 16)(216) \\
&+ (8s - 14)(225) + (8s - 16)(270) + (6s^2 - 24s + 24)(324), \\
&= 1706 + (324s - 324) + (2160s - 3240) + (1440s - 720) \\
&+ (1296s^2 - 4320s + 3456) + (1800s - 3150) + (2160s - 4320) \\
&+ (1944s^2 - 7776s + 7776), \\
&= 3240s^2 - 4212s + 1184.
\end{aligned}$$

**Theorem 3.3.** Let  $P$  be a molecular graph of RHSL network. Then modified FZCI is given by

$$\widehat{\mathcal{Z}}\mathcal{C}^*_1(P) = 396s^2 - 288s + 24.$$

**Proof:** By using Table 3 and Equation 2.3, we get

$$\begin{aligned}
\widehat{\mathcal{ZC}}^*_1(P) &= \sum_{hf \in \mathcal{L}(P)} (\varpi_P(h) + \varpi_P(f)), \\
&= |\mathcal{L}_{(5,5)}|(\varpi_P(h) + \varpi_P(f)) + |\mathcal{L}_{(5,6)}|(\varpi_P(h) + \varpi_P(f)) + |\mathcal{L}_{(5,12)}|(\varpi_P(h) + \varpi_P(f)) \\
&\quad + |\mathcal{L}_{(6,12)}|(\varpi_P(h) + \varpi_P(f)) + |\mathcal{L}_{(9,9)}|(\varpi_P(h) + \varpi_P(f)) + |\mathcal{L}_{(9,12)}|(\varpi_P(h) + \varpi_P(f)) \\
&\quad + |\mathcal{L}_{(9,15)}|(\varpi_P(h) + \varpi_P(f)) + |\mathcal{L}_{(12,12)}|(\varpi_P(h) + \varpi_P(f)) + |\mathcal{L}_{(12,15)}|(\varpi_P(h) + \varpi_P(f)) \\
&\quad + |\mathcal{L}_{(12,18)}|(\varpi_P(h) + \varpi_P(f)) + |\mathcal{L}_{(15,15)}|(\varpi_P(h) + \varpi_P(f)) + |\mathcal{L}_{(15,18)}|(\varpi_P(h) + \varpi_P(f)) \\
&\quad + |\mathcal{L}_{(18,18)}|(\varpi_P(h) + \varpi_P(f)), \\
&= 2(5 + 5) + 4(5 + 6) + 4(5 + 12) + 2(6 + 12) + (4s - 4)(9 + 9) \\
&\quad + 8(9 + 12) + (16s - 24)(9 + 15) + 2(12 + 12) + (8s - 4)(12 + 15) \\
&\quad + (6s^2 - 20s + 16)(12 + 18) + (8s - 14)(15 + 15) + (8s - 16)(15 + 18) \\
&\quad + (6s^2 - 24s + 24)(18 + 18), \\
&= 2(10) + 4(11) + 4(17) + 2(18) + (4s - 4)(18) + 8(21) + (16s - 24)(24) \\
&\quad + 2(24) + (8s - 4)(27) + (6s^2 - 20s + 16)(30) + (8s - 14)(30) \\
&\quad + (8s - 16)(33) + (6s^2 - 24s + 24)(36), \\
&= 384 + (72s - 72) + (384s - 576) + (216s - 108) + (180s^2 - 600s + 480) \\
&\quad + (240s - 420) + (264s - 528) + (216s^2 - 864s + 864), \\
&= 396s^2 - 288s + 24.
\end{aligned}$$

Next, we compute modified SZCI and modified TZCI. For this, we define the partitions of edges on the basis of CNs and degrees. From Figure 3, we obtain following partitions.

$$\begin{aligned}
\mathcal{L}_{(3,3)(5,5)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 3 \varpi(h) = 5, \deg(f) = 3 \varpi(f) = 5\}, \\
\mathcal{L}_{(3,3)(5,6)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 3 \varpi(h) = 5, \deg(f) = 3 \varpi(f) = 6\}, \\
\mathcal{L}_{(3,3)(9,9)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 3 \varpi(h) = 9, \deg(f) = 3 \varpi(f) = 9\}, \\
\mathcal{L}_{(3,6)(5,12)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 3 \varpi(h) = 5, \deg(f) = 6 \varpi(f) = 12\}, \\
\mathcal{L}_{(3,6)(6,12)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 3 \varpi(h) = 6, \deg(f) = 6 \varpi(f) = 12\}, \\
\mathcal{L}_{(3,6)(9,12)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 3 \varpi(h) = 9, \deg(f) = 6 \varpi(f) = 12\}, \\
\mathcal{L}_{(3,6)(9,15)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 3 \varpi(h) = 9, \deg(f) = 6 \varpi(f) = 15\}, \\
\mathcal{L}_{(3,6)(12,12)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 3 \varpi(h) = 12, \deg(f) = 6 \varpi(f) = 12\}, \\
\mathcal{L}_{(3,6)(12,15)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 3 \varpi(h) = 12, \deg(f) = 6 \varpi(f) = 15\}, \\
\mathcal{L}_{(3,6)(12,18)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 3 \varpi(h) = 12, \deg(f) = 6 \varpi(f) = 18\}, \\
\mathcal{L}_{(6,6)(12,15)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 6 \varpi(h) = 12, \deg(f) = 6 \varpi(f) = 15\}, \\
\mathcal{L}_{(6,6)(15,15)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 6 \varpi(h) = 15, \deg(f) = 6 \varpi(f) = 15\}, \\
\mathcal{L}_{(6,6)(15,18)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 6 \varpi(h) = 15, \deg(f) = 6 \varpi(f) = 18\}, \\
\mathcal{L}_{(6,6)(18,18)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 6 \varpi(h) = 18, \deg(f) = 6 \varpi(f) = 18\},
\end{aligned}$$

The total number of edges in each partitions are given in Table 4.

TABLE 4. Total number of edges in each partitions

$\mathcal{L}_{(deg(h),deg(f))(\varpi(h),\varpi(f))}$	$ \mathcal{L}_{(deg(h),deg(f))(\varpi(h),\varpi(f))} $
$\mathcal{L}_{(3,3)(5,5)}$	2
$\mathcal{L}_{(3,3)(5,6)}$	4
$\mathcal{L}_{(3,3)(9,9)}$	$4s - 4$
$\mathcal{L}_{(3,6)(5,12)}$	4
$\mathcal{L}_{(3,6)(6,12)}$	2
$\mathcal{L}_{(3,6)(9,12)}$	8
$\mathcal{L}_{(3,6)(9,15)}$	$16s - 24$
$\mathcal{L}_{(3,6)(12,12)}$	2
$\mathcal{L}_{(3,6)(12,15)}$	$8s - 12$
$\mathcal{L}_{(3,6)(12,18)}$	$6s^2 - 20s + 16$
$\mathcal{L}_{(6,6)(12,15)}$	8
$\mathcal{L}_{(6,6)(15,15)}$	$8s - 14$
$\mathcal{L}_{(6,6)(15,18)}$	$8s - 16$
$\mathcal{L}_{(6,6)(18,18)}$	$6s^2 - 24s + 24$

**Theorem 3.3.** Let  $P$  be a molecular graph of RHSL network. Then modified SZCI is given by

$$\widehat{\mathcal{ZC}}^*_2(P) = 2052s^2 - 1944s + 348.$$

**Proof:** By using Table 4 and Equation 2.4, we get

$$\begin{aligned} \widehat{\mathcal{ZC}}^*_2(P) &= \sum_{hf \in \mathcal{L}(P)} [deg_P(h)\varpi(f) + deg(f)\varpi(h)], \\ &= |\mathcal{L}_{(3,3)(5,5)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] + |\mathcal{L}_{(3,3)(5,6)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] \\ &\quad + |\mathcal{L}_{(3,3)(9,9)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] + |\mathcal{L}_{(3,6)(5,12)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] \\ &\quad + |\mathcal{L}_{(3,6)(6,12)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] + |\mathcal{L}_{(3,6)(9,12)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] \\ &\quad + |\mathcal{L}_{(3,6)(9,15)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] + |\mathcal{L}_{(3,6)(12,12)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] \\ &\quad + |\mathcal{L}_{(3,6)(12,15)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] + |\mathcal{L}_{(3,6)(12,18)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] \\ &\quad + |\mathcal{L}_{(6,6)(12,15)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] + |\mathcal{L}_{(6,6)(15,15)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] \\ &\quad + |\mathcal{L}_{(6,6)(15,18)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] + |\mathcal{L}_{(6,6)(18,18)}| [deg(h)\varpi(f) + deg(f)\varpi(h)], \\ &= 2 [(3)(5) + (3)(5)] + 4 [(3)(6) + (3)(5)] + (4s - 4) [(3)(9) + (3)(9)] + (4) [(3)(12) + (6)(5)] \\ &\quad + 2 [(3)(12) + (6)(6)] + 8 [(3)(12) + (6)(9)] + (16s - 24) [(3)(15) + (6)(9)] + (2) [(3)(12) + (6)(12)] \\ &\quad + (8s - 12) [(3)(15) + (6)(12)] + (6s^2 - 20s + 16) [(3)(18) + (6)(12)] + (8) [(6)(15) + (6)(12)] \\ &\quad + (8s - 14) [(6)(15) + (6)(15)] + (8s - 16) [(6)(18) + (6)(15)] + (6s^2 - 24s + 24) [(6)(18) + (6)(18)], \\ &= 2 [15 + 15] + 4 [18 + 15] + (4s - 4) [27 + 27] + (4) [36 + 30] + 2 [36 + 36] \\ &\quad + 8 [36 + 54] + (16s - 24) [45 + 54] + (2) [36 + 72] + (8s - 12) [45 + 72] \\ &\quad + (6s^2 - 20s + 16) [54 + 72] + (8) [90 + 72] + (8s - 14) [90 + 90] \\ &\quad + (8s - 16) [108 + 90] + (6s^2 - 24s + 24) [108 + 108], \\ &= 2 [30] + 4 [33] + (4s - 4) [54] + (4) [66] + 2 [72] + 8 [90] + (16s - 24) [99] \end{aligned}$$

$$\begin{aligned}
& +(2) [108] + (8s - 12) [117] + (6s^2 - 20s + 16) [126] + (8) [162] \\
& +(8s - 14) [180] + (8s - 16) [198] + (6s^2 - 24s + 24) [216], \\
= & 2832 + (216s - 216) + (1584s - 2376) + (936s - 1404) + (756s^2 - 2520s + 2016) \\
& +(1440s - 2520) + (1584s - 3168) + (1296s^2 - 5184s + 5184), \\
& = 2052s^2 - 1944s + 348.
\end{aligned}$$

**Theorem 3.4.** *Let  $P$  be a molecular graph of RHSL network. Then modified TZCI is given by*

$$\widehat{\mathcal{ZC}}^*_3(P) = 2160s^2 - 1944s + 288.$$

**Proof:** By using Table 4 and Equation 2.5, we get

$$\begin{aligned}
\widehat{\mathcal{ZC}}^*_3(P) &= \sum_{hf \in \mathcal{L}(P)} [deg(h)\varpi(h) + deg(f)\varpi(f)], \\
&= |\mathcal{L}_{(3,3)(5,5)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] + |\mathcal{L}_{(3,3)(5,6)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] \\
&+ |\mathcal{L}_{(3,3)(9,9)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] + |\mathcal{L}_{(3,6)(5,12)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] \\
&+ |\mathcal{L}_{(3,6)(6,12)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] + |\mathcal{L}_{(3,6)(9,12)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] \\
&+ |\mathcal{L}_{(3,6)(9,15)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] + |\mathcal{L}_{(3,6)(12,12)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] \\
&+ |\mathcal{L}_{(3,6)(12,15)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] + |\mathcal{L}_{(3,6)(12,18)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] \\
&+ |\mathcal{L}_{(6,6)(12,15)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] + |\mathcal{L}_{(6,6)(15,15)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] \\
&+ |\mathcal{L}_{(6,6)(15,18)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] + |\mathcal{L}_{(6,6)(18,18)}| [deg(h)\varpi(h) + deg(f)\varpi(f)], \\
= & 2 [(3)(5) + (3)(5)] + 4 [(3)(5) + (3)(6)] + (4s - 4) [(3)(9) + (3)(9)] + (4) [(3)(5) + (6)(12)] \\
& + 2 [(3)(6) + (6)(12)] + 8 [(3)(9) + (6)(12)] + (16s - 24) [(3)(9) + (6)(15)] + (2) [(3)(12) + \\
& (6)(12)] + (8s - 12) [(3)(12) + (6)(15)] + (6s^2 - 20s + 16) [(3)(12) + (6)(18)] + (8) \\
& [(6)(12) + (6)(15)] + (8s - 14) [(6)(15) + (6)(15)] + (8s - 16) [(6)(15) + (6)(18)] \\
& + (6s^2 - 24s + 24) [(6)(18) + (6)(18)] \\
= & 2 [15 + 15] + 4 [15 + 18] + (4s - 4) [27 + 27] + (4) [15 + 72] + 2 [18 + 72] \\
& + 8 [27 + 72] + (16s - 24) [27 + 90] + (2) [36 + 72] + (8s - 12) [36 + 90] \\
& + (6s^2 - 20s + 16) [36 + 108] + (8) [72 + 90] + (8s - 14) [90 + 90] + (8s - 16) [90 + 108] \\
& + (6s^2 - 24s + 24) [108 + 108], \\
= & 2 [30] + 4 [33] + (4s - 4) [54] + (4) [87] + 2 [90] + 8 [99] + (16s - 24) \\
& [117] + (2) [108] + (8s - 12) [126] + (6s^2 - 20s + 16) [144] + (8) [162] \\
& + (8s - 14) [180] + (8s - 16) [198] + (6s^2 - 24s + 24) [216], \\
= & 3024 + (216s - 216) + (1872s - 2808) + (1008s - 1512) + (864s^2 - 2880s + 2304) \\
& +(1440s - 2520) + (1584s - 3168) + (1296s^2 - 5184s + 5184), \\
& = 2160s^2 - 1944s + 288.
\end{aligned}$$

#### 4. ZCIs OF RHOX NETWORK

In this section, we calculate the ZCIs for the RHOX network. Let  $P = RHOX(s)$ , be a molecular graph RHOX network, where  $s \geq 2$  is the dimension of the network. In Figure 4, Figure 5 and Figure 6, we represent the molecular graph of  $P = (\mathcal{H}, \mathcal{L})$  of  $RHOX(s)$  for  $s = 2, 3, 4$  by labeling the vertices with their CNs. For this, let us define the partitions of the vertices which are based on the CNs of the vertices. From Figure 6, we can see that there are five vertex-based partitions as given below.

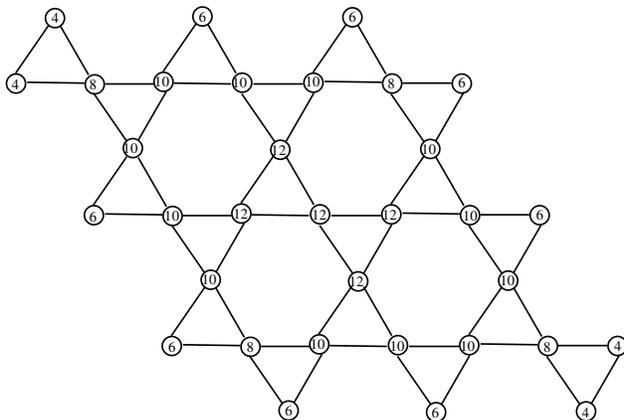


FIGURE 4. RHOX(3) along with the CN each vertex.

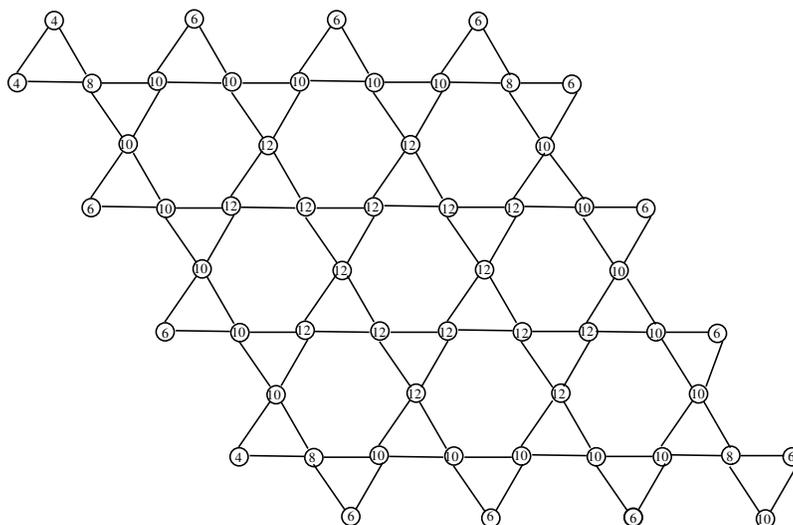


FIGURE 5. RHOX(4) along with the CN each vertex

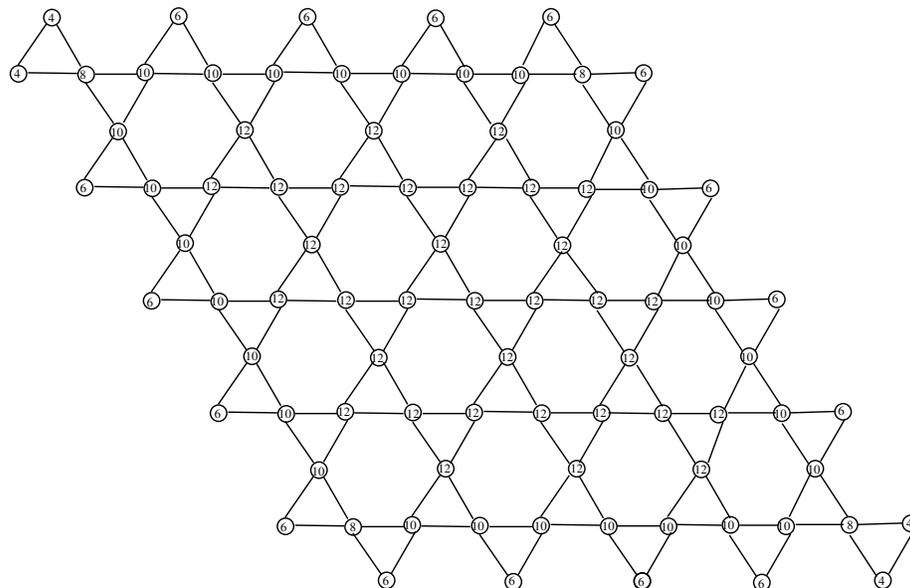


FIGURE 6. RHOX(5) along with the CN each vertex

$$\begin{aligned} \mathcal{H}_4 &= \{h \in \mathcal{H}(P) : \varpi(h) = 4\}, \\ \mathcal{H}_6 &= \{h \in \mathcal{H}(P) : \varpi(h) = 6\}, \\ \mathcal{H}_8 &= \{h \in \mathcal{H}(P) : \varpi(h) = 8\}, \\ \mathcal{H}_{10} &= \{h \in \mathcal{H}(P) : \varpi(h) = 10\}, \\ \mathcal{H}_{12} &= \{h \in \mathcal{H}(P) : \varpi(h) = 12\}, \\ \mathcal{H}_{15} &= \{h \in \mathcal{H}(P) : \varpi(h) = 15\}, \end{aligned}$$

The total number of vertices in each partitions are given in Table 5. By adding all the vertices of each partition

TABLE 5. Total number of vertices in each partition

$\mathcal{H}_{\varpi(h)}$	$ \mathcal{H}_{\varpi(h)} $
$\mathcal{H}_4$	4
$\mathcal{H}_6$	$4s - 4$
$\mathcal{H}_8$	4
$\mathcal{H}_{10}$	$8s - 12$
$\mathcal{H}_{12}$	$3s^2 - 10s + 8$

gives the total number of vertices of  $ZNOX(s)$  network. In the similar way, we define the edge partitions.

From Figure 3, we can see that there are thirteen edge based partitions as given below.

$$\begin{aligned}\mathcal{L}_{(4,4)} &= \{hf \in \mathcal{L}(P) : \varpi(h) = 4, \varpi(f) = 4\}, \\ \mathcal{L}_{(4,8)} &= \{hf \in \mathcal{L}(P) : \varpi(h) = 4, \varpi(f) = 8\} \\ \mathcal{L}_{(6,8)} &= \{hf \in \mathcal{L}(P) : \varpi(h) = 6, \varpi(f) = 8\}, \\ \mathcal{L}_{(6,10)} &= \{hf \in \mathcal{L}(P) : \varpi(h) = 6, \varpi(f) = 10\} \\ \mathcal{L}_{(8,10)} &= \{hf \in \mathcal{L}(P) : \varpi(h) = 8, \varpi(f) = 10\}, \\ \mathcal{L}_{(10,10)} &= \{hf \in \mathcal{L}(P) : \varpi(h) = 10, \varpi(f) = 10\}, \\ \mathcal{L}_{(10,12)} &= \{hf \in \mathcal{L}(P) : \varpi(h) = 10, \varpi(f) = 12\}, \\ \mathcal{L}_{(12,12)} &= \{hf \in \mathcal{L}(P) : \varpi(h) = 12, \varpi(f) = 12\},\end{aligned}$$

The total count of the above classified vertices are given in Table 6.

TABLE 6. Count of CN-based classified vertices of  $P$

$\mathcal{L}_{(h,f)}$	$ \mathcal{L}_{(h,f)} $
$\mathcal{L}_{(4,4)}$	2
$\mathcal{L}_{(4,8)}$	4
$\mathcal{L}_{(6,8)}$	4
$\mathcal{L}_{(6,10)}$	$8s-12$
$\mathcal{L}_{(8,10)}$	8
$\mathcal{L}_{(10,10)}$	$8s-14$
$\mathcal{L}_{(10,12)}$	$8s - 16$
$\mathcal{L}_{(12,12)}$	$6s^2 - 24s + 24$

**Theorem 4.1.** *Let  $P$  be a molecular graph of RHOX network. Then FZCI is given by*

$$\widehat{\mathcal{Z}}\mathcal{C}_1(P) = 432s^2 - 496s + 128.$$

**Proof:** By using Table 5 and Equation 2. 1 , we get

$$\begin{aligned}\widehat{\mathcal{Z}}\mathcal{C}_1(P) &= \sum_{h \in \mathcal{H}(P)} (\varpi_P(h))^2, \\ &= |\mathcal{H}_4|(\varpi_P(h))^2 + |\mathcal{H}_6|(\varpi_P(h))^2 + |\mathcal{H}_8|(\varpi_P(h))^2 \\ &\quad + |\mathcal{H}_{10}|(\varpi_P(h))^2 + |\mathcal{H}_{12}|(\varpi_P(h))^2, \\ &= 4(4)^2 + (4s-4)(6)^2 + 4(8)^2 + (8s-12)(10)^2 \\ &\quad + (3s^2-10s+8)(12)^2, \\ &= 4(16) + (4s-4)(36) + 4(64) + (8s-12)(100) + (3s^2-10s+8)(144), \\ &= 320 + (144s-144) + (800s-1200) + (432s^2-1440s+1152), \\ &= 432s^2 - 496s + 128.\end{aligned}$$

**Theorem 4.2.** Let  $P$  be a molecular graph of RHOX network. Then SZCI is given by

$$\widehat{\mathcal{ZC}}_2(P) = 864s^2 - 1216s + 408.$$

**Proof:** By using Table 6 and Equation 2.2, we get

$$\begin{aligned} \widehat{\mathcal{ZC}}_2(P) &= \sum_{hf \in \mathcal{L}(P)} (\varpi_P(h) \times \varpi_P(f)), \\ &= |\mathcal{L}_{(4,4)}|(\varpi_P(h) \times \varpi_P(f)) + |\mathcal{L}_{(4,8)}|(\varpi_P(h) \times \varpi_P(f)) + |\mathcal{L}_{(6,8)}|(\varpi_P(h) \times \varpi_P(f)) \\ &+ |\mathcal{L}_{(6,10)}|(\varpi_P(h) \times \varpi_P(f)) + |\mathcal{L}_{(8,10)}|(\varpi_P(h) \times \varpi_P(f)) + |\mathcal{L}_{(10,10)}|(\varpi_P(h) \times \varpi_P(f)) \\ &+ |\mathcal{L}_{(10,12)}|(\varpi_P(h) \times \varpi_P(f)) + |\mathcal{L}_{(12,12)}|(\varpi_P(h) \times \varpi_P(f)), \\ &= 2(4 \times 4) + 4(4 \times 8) + 4(6 \times 8) + (8s - 12)(6 \times 10) + 8(8 \times 10) + (8s - 14)(10 \times 10) \\ &+ (8s - 16)(10 \times 12) + (6s^2 - 24s + 24)(12 \times 12), \\ &= 2(16) + 4(32) + 4(48) + (8s - 12)(60) + 8(80) + (8s - 14)(100) \\ &+ (8s - 16)(120) + (6s^2 - 24s + 24)(144), \\ &= 992 + (480s - 720) + (800s - 1400) + (960s - 1920) + (864s^2 - 3456s + 3456), \\ &= 864s^2 - 1216s + 408. \end{aligned}$$

**Theorem 4.3.** Let  $P$  be a molecular graph of RHOX network. Then modified FZCI is given by

$$\widehat{\mathcal{ZC}}^*_1(P) = 144s^2 - 83s + 16.$$

**Proof:** By using Table 6 and Equation 2.3, we get

$$\begin{aligned} \widehat{\mathcal{ZC}}^*_1(P) &= \sum_{hf \in \mathcal{L}(P)} (\varpi_P(h) + \varpi_P(f)), \\ &= |\mathcal{L}_{(4,4)}|(\varpi_P(h) + \varpi_P(f)) + |\mathcal{L}_{(4,8)}|(\varpi_P(h) + \varpi_P(f)) + |\mathcal{L}_{(6,8)}|(\varpi_P(h) + \varpi_P(f)) \\ &+ |\mathcal{L}_{(6,10)}|(\varpi_P(h) + \varpi_P(f)) + |\mathcal{L}_{(8,10)}|(\varpi_P(h) + \varpi_P(f)) + |\mathcal{L}_{(10,10)}|(\varpi_P(h) + \varpi_P(f)) \\ &+ |\mathcal{L}_{(10,12)}|(\varpi_P(h) + \varpi_P(f)) + |\mathcal{L}_{(12,12)}|(\varpi_P(h) + \varpi_P(f)), \\ &= 2(4 + 4) + 4(4 + 8) + 4(6 + 8) + (8s - 12)(6 + 10) + 8(8 + 10) + (8s - 14)(10 + 10) \\ &+ (8s - 16)(10 + 12) + (6s^2 - 24s + 24)(12 + 12), \\ &= 2(8) + 4(12) + 4(14) + (8s - 12)(16) + 8(18) + (8s - 14)(20) \\ &+ (8s - 16)(22) + (6s^2 - 24s + 24)(24), \\ &= 264 + (128s - 192) + (160s - 280) + (176s - 352) + (144s^2 - 547s + 576), \\ &= 144s^2 - 83s + 16. \end{aligned}$$

Next, we compute modified SZCI and modified TZCI. For this we define the partitions of edges on the basis of CNs and degrees. From Figure 6, we obtain following partitions.

$$\begin{aligned} \mathcal{L}_{(2,2)(4,4)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 2 \varpi(h) = 4, \deg(f) = 2 \varpi(f) = 4\}, \\ \mathcal{L}_{(2,4)(4,8)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 2 \varpi(h) = 4, \deg(f) = 4 \varpi(f) = 8\}, \\ \mathcal{L}_{(2,4)(6,8)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 2 \varpi(h) = 6, \deg(f) = 4 \varpi(f) = 8\}, \\ \mathcal{L}_{(2,4)(6,10)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 2 \varpi(h) = 6, \deg(f) = 4 \varpi(f) = 10\}, \\ \mathcal{L}_{(4,4)(8,10)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 4 \varpi(h) = 8, \deg(f) = 4 \varpi(f) = 10\}, \\ \mathcal{L}_{(4,4)(10,10)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 4 \varpi(h) = 10, \deg(f) = 4 \varpi(f) = 10\}, \\ \mathcal{L}_{(4,4)(10,12)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 4 \varpi(h) = 10, \deg(f) = 4 \varpi(f) = 12\}, \\ \mathcal{L}_{(4,4)(12,12)} &= \{hf \in \mathcal{L}(P) : \deg(h) = 4 \varpi(h) = 12, \deg(f) = 4 \varpi(f) = 12\}. \end{aligned}$$

The total number of edges in each partitions are given in Table 7.

TABLE 7. Total number of edges in each partitions

$\mathcal{L}_{(deg(h),deg(f))(\varpi(h),\varpi(f))}$	$ \mathcal{L}_{(deg(h),deg(f))(\varpi(h),\varpi(f))} $
$\mathcal{L}_{(2,2)(4,4)}$	2
$\mathcal{L}_{(2,4)(4,8)}$	2
$\mathcal{L}_{(2,4)(6,8)}$	4
$\mathcal{L}_{(2,4)(6,10)}$	$8s-12$
$\mathcal{L}_{(4,4)(8,10)}$	8
$\mathcal{L}_{(4,4)(10,10)}$	$8s-14$
$\mathcal{L}_{(4,4)(10,12)}$	$8s-16$
$\mathcal{L}_{(4,4)(12,12)}$	$6s^2 - 24s + 24$

**Theorem 4.4.** Let  $P$  be a molecular graph of RHOX network. Then modified SZCI is given by

$$\widehat{\mathcal{ZC}}^*_2(P) = 576s^2 - 608s + 80.$$

**Proof:** By using Table 4 and Equation 2. 4 , we get

$$\begin{aligned} \widehat{\mathcal{ZC}}^*_2(P) &= \sum_{hf \in \mathcal{L}(P)} [deg(h)\varpi(f) + deg(f)\varpi(h)], \\ &= |\mathcal{L}_{(2,2)(4,4)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] + |\mathcal{L}_{(2,4)(4,8)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] \\ &\quad + |\mathcal{L}_{(2,4)(6,8)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] + |\mathcal{L}_{(2,4)(6,10)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] \\ &\quad + |\mathcal{L}_{(4,4)(8,10)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] + |\mathcal{L}_{(4,4)(10,10)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] \\ &\quad + |\mathcal{L}_{(4,4)(10,12)}| [deg(h)\varpi(f) + deg(f)\varpi(h)] + |\mathcal{L}_{(4,4)(12,12)}| [deg(h)\varpi(f) + deg(f)\varpi(h)], \\ &= 2 [(2)(4) + (2)(4)] + 2 [(2)(8) + (4)(4)] + 4 [(2)(8) + (4)(6)] + (8s - 12) [(2)(10) + (4)(6)] \\ &\quad + 8 [(4)(10) + (4)(8)] + (8s - 14) [(4)(10) + (4)(10)] + (8s - 16) [(4)(12) + (4)(10)] \\ &\quad + (6s^2 - 24s + 24) [(4)(12) + (4)(12)], \\ &= 2 [8 + 8] + 2 [16 + 16] + 4 [16 + 24] + (8s - 12) [20 + 24] + 8 [40 + 32] \\ &\quad + (8s - 14) [40 + 40] + (8s - 16) 2 [48 + 40] + (6s^2 - 24s + 24) [48 + 48], \\ &= 2 [16] + 2 [32] + 4 [40] + (8s - 12) [44] + 8 [72] + (8s - 14) [80] + (8s - 16) [88] \\ &\quad + (6s^2 - 24s + 24) [96], \\ &= 832 + (352s - 528) + (640s - 1120) + (704s - 1408) + (576s^2 - 2304s + 2304), \\ &= 576s^2 - 608s + 80. \end{aligned}$$

**Theorem 4.5.** Let  $P$  be a molecular graph of RHOX network. Then modified TZCI is given by

$$\widehat{\mathcal{ZC}}^*_3(P) = 576s^2 - 544s + 16.$$

**Proof:** By using Table 4 and Equation 2.5, we get

$$\begin{aligned}
 \widehat{ZC}_3^*(P) &= \sum_{hf \in \mathcal{L}(P)} [deg(h)\varpi(h) + deg(f)\varpi(f)], \\
 &= |\mathcal{L}_{(2,2)(4,4)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] + |\mathcal{L}_{(2,4)(4,8)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] \\
 &+ |\mathcal{L}_{(2,4)(6,8)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] + |\mathcal{L}_{(2,4)(6,10)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] \\
 &+ |\mathcal{L}_{(4,4)(8,10)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] + |\mathcal{L}_{(4,4)(10,10)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] \\
 &+ |\mathcal{L}_{(4,4)(10,12)}| [deg(h)\varpi(h) + deg(f)\varpi(f)] + |\mathcal{L}_{(4,4)(12,12)}| [deg(h)\varpi(h) + deg(f)\varpi(f)], \\
 &= 2[(2)(4) + (2)(4)] + 2[(2)(4) + (4)(8)] + 4[(2)(6) + (4)(8)] \\
 &+ (8s - 12)[(2)(6) + (4)(10)] + 8[(4)(8) + (4)(10)] + (8s - 14)[(4)(10) + (4)(10)] \\
 &+ (8s - 16)[(4)(10) + (4)(12)] + (6s^2 - 24s + 24)[(4)(12) + (4)(12)], \\
 &= 2[8 + 8] + 2[8 + 32] + 4[12 + 32] + (8s - 12)[12 + 40] + 8[32 + 40] \\
 &+ (8s - 14)[40 + 40] + (8s - 16)[40 + 48] + (6s^2 - 24s + 24)[48 + 48], \\
 &= 2[16] + 2[40] + 4[44] + (8s - 12)[52] + 8[72] \\
 &+ (8s - 14)[80] + (8s - 16)[88] + (6s^2 - 24s + 24)[96], \\
 &= 864 + (416s - 624) + (640s - 1120) + (704s - 1408) + (576s^2 - 2304s + 2304), \\
 &= 576s^2 - 544s + 16.
 \end{aligned}$$

### 5. COMPARATIVE ANALYSIS

In this part, we individually compare the results of all the calculated ZCIs for the rhombus silicate and rhombus oxide networks using line graphs. In sections 3 and 4, we have computed the general results of the *RHSL* and *RHOX* in terms of  $s$  where  $s$  is the dimension. In Table 8 and Table 9 we have computed the values of ZCIs of RHSL and RHOX network for  $s = 1, 2, 3, \dots, 8$ , respectively. In Figure 7, we have taken the values of  $s$  along the horizontal axis and the computed values of the indices along the vertical axis. From Figure 7, it is clear that SZCI attains the higher values for the RHSL network. Similarly in Figure 8, we can see that again SZCI attains the higher values for RHOX network.

TABLE 8. Computed values of ZCIs for  $s = 1, 2, 3, \dots, 10$

ZCIs	$s = 1$	$s = 2$	$s = 3$	$s = 4$	$s = 5$	$s = 6$	$s = 7$	$s = 8$	$s = 9$	$s = 10$
FZCI	172	2584	7516	14968	24940	37432	52444	69976	90028	112600
SZCI	212	5720	17708	36176	61124	92552	130460	174848	225716	283064
Modified FZCI	132	1032	2724	5208	8484	12552	17412	23064	29508	36744
Modified SZCI	456	4668	12984	25404	41928	62556	87288	116124	149064	186108
Modified SZCI	504	5040	13896	27072	44568	66384	92520	122976	157752	196848

TABLE 9. Computed values of ZCIs for  $s = 1, 2, 3, \dots, 10$

ZCIs	$s = 1$	$s = 2$	$s = 3$	$s = 4$	$s = 5$	$s = 6$	$s = 7$	$s = 8$	$s = 9$	$s = 10$
FZCI	64	864	2528	5056	8448	12704	17824	23808	30656	38368
SZCI	56	1432	4536	9368	15928	24216	34232	45976	59448	74648
Modified FZCI	77	426	1063	1988	3201	4702	6491	8568	10933	13586
Modified SZCI	48	1168	3440	6864	11440	17168	24048	32080	41264	51600
Modified SZCI	48	1232	3568	7056	11696	17488	24432	32528	41776	52176

From Figure 7 and Figure 8, it can be seen that SZCI has the maximum values for RHSL and RHOX networks. In Figure 9, we compare the RHSL and RHOX networks.

From Figure 9, it is clear that the computed values of SZCI for the RHSL network show a clear difference with the increasing values of  $s$  than that of RHOX network.

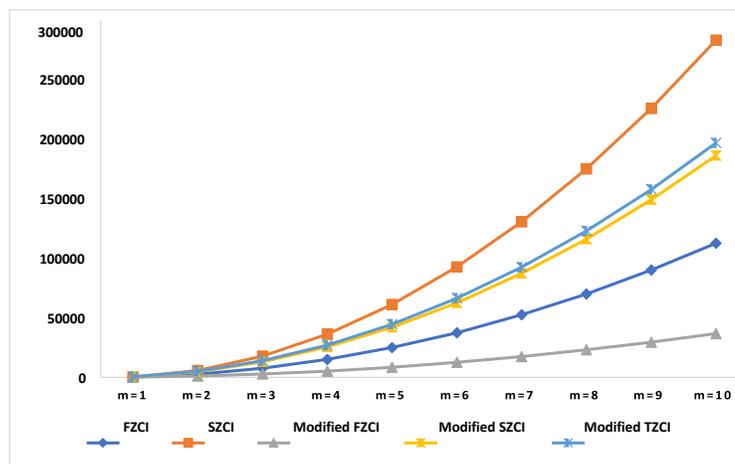


FIGURE 7. Comparison of the TIs of the rhombus silicate network.

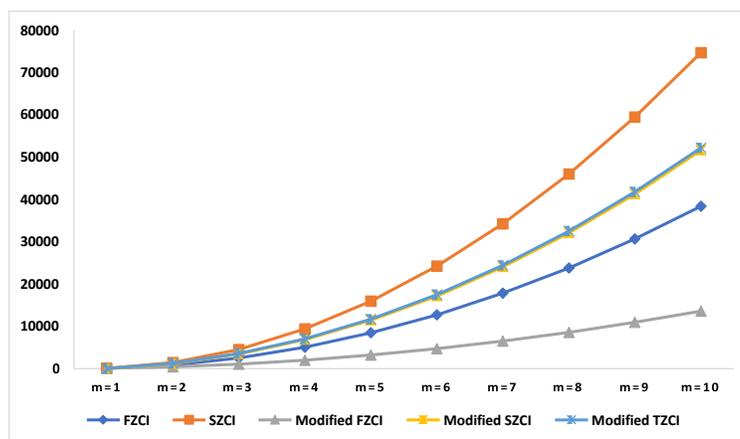


FIGURE 8. Comparison of the TIs of the rhombus oxide network.

## 6. CONCLUSION

A topological index (TI) is a numerical value that characterizes the topology of a chemical structure. Zagreb connection indices are newly introduced indices that are widely utilized in defining the properties of chemical structures. In this paper, we have computed ZCIs of two significant chemical structures, namely, rhombus silicate and rhombus oxide network. We have calculated FZCI, SZCI, Modified FZCI, Modified SZCI, and Modified TZCI of rhombus silicate and rhombus oxide networks. Furthermore, we have compared these structures based on their calculated general results. These findings are novel and contribute to majoring in network science and provide

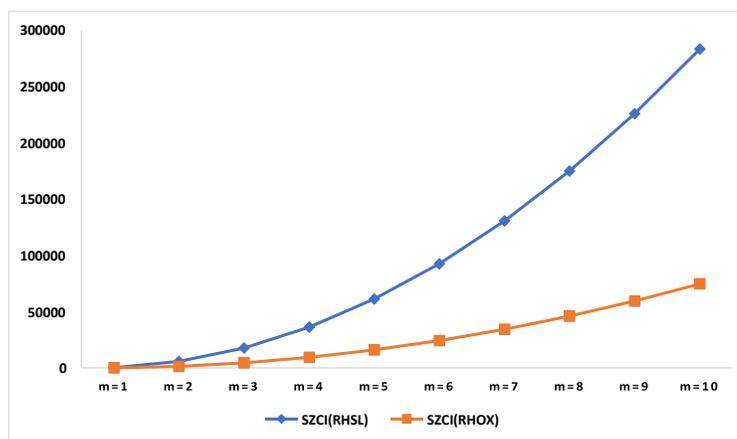


FIGURE 9. Comparison of RHSL and RHOX network.

a foundation for understanding the deep topology of these critical networks. Moreover, these findings are eye-opening for the scientists on how these networks may be built and how good are their topological features.

**Data Availability:** The data supporting the findings are included in this article. However, for additional details, the reader may contact the corresponding author.

**Conflict of Interest** The author declare no conflict of interest for this article.

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