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Research Article

On the Comparative Analysis among Topological Indices for Rhombus Silicate and Oxide Structures

Aqsa Sattar,[1] **Muhammad Javaid**,[1] **and Mamo Abebe Ashebo**[2]

[1]*Department of Mathematics, School of Science, University of Management and Technology, Lahore 54770, Pakistan*
[2]*Department of Mathematics, Wollega University, Nekemte, Ethiopia*

Correspondence should be addressed to Mamo Abebe Ashebo; mamoabebe37@gmail.com

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A topological index (TI) is a numeric digit that signalizes the whole chemical structure of a molecular network. TIs are helpful in predicting the bioactivity of molecular substances in investigations of quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR). TIs correlate various chemical and physical attributes of chemical substances such as melting and freezing point, strain energy, stability, temperature, volume, density, and pressure. There are several distance-based descriptors available in the literature, but connection-based TIs are considered more effective than degree-based TIs in measuring the chemical characteristics of molecular compounds. The present study focuses on computing the connection-based TIs for the most significant type of chemical structures, namely, rhombus silicate and rhombus oxide networks. At the end, we compare these structures on the basis of their computed result.

1. Introduction

Graph theory (GT) is an important branch of mathematics that studies the objects and relationships between them. The concept of GT was first introduced by a Swiss mathematician Leonhard Euler in 1735 when he solved the famous Königsberg Bridge problem. GT has a wide range of applications in different areas such as software engineering, computer science, data structures, graph coloring, website design, operating systems, networking, and many others. A graph consists of points called vertices and lines connecting those points called edges. Chemical GT is a branch of mathematical chemistry that models molecular chemical structures using graphs. In chemical GT, molecular compounds are represented by molecular graphs. A molecular graph, in terms of GT, is a depiction of a molecular structural formula where atoms are represented by vertices and bonds by edges. Computation of topological indices (TIs) is a subtopic of chemical GT that connects various physicochemical features of the underlying chemical substance. In simple words, TIs convert the molecular structural information into a numeric value. TIs are widely used in toxicology for relational analysis, as well as in environmental and theoretical chemistry. They have a vast range of applications in various other fields of science, such as predicting the chemical properties of molecular structures and bioactivity of molecular compounds, which is critical in medication design and development. By analyzing the TIs of diverse substances, researchers can find molecules with desired biological characteristics, resulting in the creation of novel medications. They can also be used to predict various material characteristics and can assist in forecasting chemical parameters such as melting point, freezing point, strain energy, stability, temperature, volume, density, and pressure. This knowledge is useful for creating materials with certain properties for a variety of uses, such as the manufacturing industry. They are extensively utilized in the study of quantitative structure-activity and property relationships [1].

TIs are categorized into three main classes, namely, distance-based TI, degree-based TI, and spectrum-based TI. Wiener [2] initiated the novel conception of distance-based TI. The innovative conception of the first degree-based Zagreb index (ZI) was initiated by Gutman and Trinajstic

[3]. This development gave a way to researchers to investigate more such TIs. After this discovery, a number of TIs were explored by distinct scientists and they utilized these new TIs in exploring the physical and chemical properties of molecular compounds [4, 5]. In 1998, the atom-bond connectivity (ABC) index which is a significant type of TI was given by Estrada et al. [6]. Furthermore, its fourth version (ABC_4I) was introduced by Ghorbani et al. [7]. Vukicevic and Furtula [8] investigated another important type of index named as geometric-arithmetic (GA) index in 2009. Furthermore, Garaovoc et al. [9] checked the chemical properties of dendrimers by utilizing a new index named as the fifth version of the GA index. Vukicevic [10] investigated the novel idea of the symmetric division degree (SDD) index in 2010. Das et al. [11] found the bounds of the SDD index of graphs. Later on, Furtula et al. [12] introduced the augmented Zagreb index (AZI). The novel conception of the harmonic index (HI) was given by Fajtlowicz [13]. The idea of the inverse sum (IS) index was initiated by Vukicevic and Gasperov [14]. Matejic et al. [15] found the upper bounds of the IS index of graphs. Furthermore, Shirdel et al. [16] introduced an innovative idea of hyper-ZI (HZI). Furtula et al. [17] computed the atom-bond connectivity index of trees. Gao and Farahani [18] calculated the HZI of some dendrimer nanostars.

All these introduced ZIs are degree-based ZIs which depend upon the degree of the vertices of molecular graphs. Recently, connection number (CN-) based ZIs are investigated by Ali and Trinajstic [19] which depend upon the CN of the vertices. A CN is a count of those vertices which are at distance two from a certain vertex. CN-based ZI (ZCI), instead of degree-based ZIs has a wide range of applicability in finding the physical and chemical attributes of chemical substances. According to scientists, Zagreb connection indices (ZCIs) provide a better platform than the other classical ZIs to measure the physical and chemical attributes of molecular chemical structures. They examined the applicability of ZCIs on octane isomers. Sattar et al. [20, 21] calculated the novel ZCIs for some zinc oxide and silicate networks. For details about Zagreb connection indices, the readers are referred to [22, 23]. Fatima et al. [24] computed ZCIs of some chemical structures. Furthermore, Kamran et al. computed the M polynomial and TIs of phenol formaldehyde [25]. Besides these, many chemical structures have been characterized by different researchers as one can see [26–28].

The methodology involved in this study encompasses the computation of connection-based topological indices (TIs), namely, ABBI, GAI, AZI, SDI, HI, ISI, and HZI for prominent chemical structures, specifically rhombus silicate and rhombus oxide networks. The study utilizes distance-based descriptors, focusing on the effectiveness of connection-based TIs compared to degree-based TIs in measuring the chemical characteristics of molecular compounds. The computed results are then employed to conduct a comparative analysis of these chemical structures. This research article is organized as follows: Section 2 involves some basic definitions and formulas which are used for the computation of main results. Section 3 covers the main results for the rhombus silicate network. In Section 4, we compute the ZIs for the rhombus oxide network. In Section 5, a comparative analysis among computed TIs of RHSL and RHOX networks and between these networks is presented. Section 6 covers the conclusions.

2. Basic Definitions

Suppose that $\mathbb{G} = (\mathscr{P}(\mathbb{G}), \mathscr{Q}(\mathbb{G}))$ is a network, where $\mathscr{P}(\mathbb{G})\, \mathscr{Q}(\mathbb{G})$ are a set of nodes (vertices) and edges. The count of those nodes which are at distance one from vertex t is said to be the degree of that node t, and the count of those nodes which are at distance two is referred to as the connection number (CN) of node t. We consider $e = (t, k)$, where $t, k \in \mathscr{P}(\mathbb{G})$ is an edge, then the degree of the e is $\deg(e) = \deg(t) + \deg(k) - 2$. Degree-based indices along with their formulas are given in Table 1. CN-based indices along with their formulas defined by Sattar and Javaid [29] are in Table 2.

3. Construction of RHSL and RHOX Networks

In this section, we will look at how to build RHSL and RHOX networks. By far, silicate is the most intriguing class of minerals. These networks are produced when metal carbonates and metal oxides are fused with sand. As a basic unit, SiO_4 tetrahedron is found in all silicates. In chemistry, the vertices at the corners of SiO_4 tetrahedron depict oxygen ions, while the vertices at the center depict silicon ions. In GT, the corner vertices are referred to as oxygen nodes, while the center vertices are referred to as silicon nodes. Different silicate structures can be obtained by arranging the tetrahedron silicate in different ways. Similarly, distinct silicate structures build different silicate networks. Figure 1 depicts the RHSL network of dimension 3, i.e., RHSL(3). By deleting silicon ions from the RHSL network, we obtained the RHOX network as depicted in Figure 2. In the present study, we denote the RHSL and RHOX networks of dimension m by $RHSL(m)$ and $RHOX(m)$. In general, the total count of vertices and edges in $RHSL(m)$ are $5m^2 + 2m$ and $12m^2$, respectively. Furthermore, the total count of vertices and edges in the $RHOX(m)$ network are $3m^2 + 2m$ and $6m^2$, respectively.

4. CN-Based ZIs of the RHSL Network

In this section, we calculate the CN-based ZIs of RHSL. Let $\Upsilon = RHSL(m)$ be a molecular graph RHSL network, where $m \geq 2$ is the dimension of the network. In Figures 3–5, we represent the molecular graph of $\Upsilon = (\mathscr{P}, \mathscr{Q})$ of $\mathrm{RHSL}(m)$ for $m = 2, 3, 4$ by labeling the vertices with their CNs.

Table 1: Topological indices on the basis of degrees of nodes.

Formulas	Name of indices	Acronyms
$\sum_{t,k\in \mathcal{Q}(\mathbb{G})}\sqrt{\frac{\deg(t)+\deg(k)-2}{\deg(t)\times\deg(k)}}$	Atom-bond connectivity index [6]	ABCI
$\sum_{t,k\in \mathcal{Q}(\mathbb{G})}\frac{2\sqrt{\deg(t)\deg(k)}}{\deg(t)+\deg(k)}$	Geometric-arithmetic index [8]	GAI
$\sum_{t,k\in \mathcal{Q}(\mathbb{G})}\left[\frac{\deg(t)\times\deg(k)}{\deg(t)+\deg(k)-2}\right]^3$	Augmented Zagreb index [12]	AZI
$\sum_{t,k\in \mathcal{Q}(\mathbb{G})}\left[\frac{\min(\deg(t),\deg(k))}{\max(\deg(t),\deg(k))}+\frac{\max(\deg(t),\deg(k))}{\min(\deg(t),\deg(k))}\right]$	Symmetry division degree index [8]	SDDI
$\sum_{t,k\in E(\mathbb{G})}\frac{2}{(\deg(t)+\deg(k))}$	Harmonic index [13]	HI
$\sum_{t,k\in \mathcal{Q}(\mathbb{G})}\frac{\deg(t)\times\deg(k)}{(\deg(t)+\deg(k))}$	Inverse sum index [14]	ISI
$\sum_{t,k\in \mathcal{Q}(\mathbb{G})}[\deg(t)+\deg(k)]^2$	Hyper-Zagreb index [16]	HZI

Table 2: Topological indices on the basis of CN of nodes.

Formulas	Name of indices	Acronyms
$\sum_{t,k\in \mathcal{Q}(\mathbb{G})}\sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}}$	Atom-bond connectivity connection index [29]	ABCCI
$\sum_{t,k\in \mathcal{Q}(\mathbb{G})}\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}$	Geometric-arithmetic connection index [29]	GACI
$\sum_{t,k\in \mathcal{Q}(\mathbb{G})}\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3$	Augmented Zagreb connection index [29]	AZCI
$\sum_{t,k\in \mathcal{Q}(\mathbb{G})}\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]$	Symmetry division connection index [29]	SDCI
$\sum_{t,k\in E(\mathbb{G})}\frac{2}{(\alpha(t)+\alpha(k))}$	Harmonic connection index [29]	HCI
$\sum_{t,k\in \mathcal{Q}(\mathbb{G})}\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))}$	Inverse sum connection index [29]	ISCI
$\sum_{t,k\in \mathcal{Q}(\mathbb{G})}[\alpha(t)+\alpha(k)]^2$	Hyper-Zagreb connection index [29]	HZCI

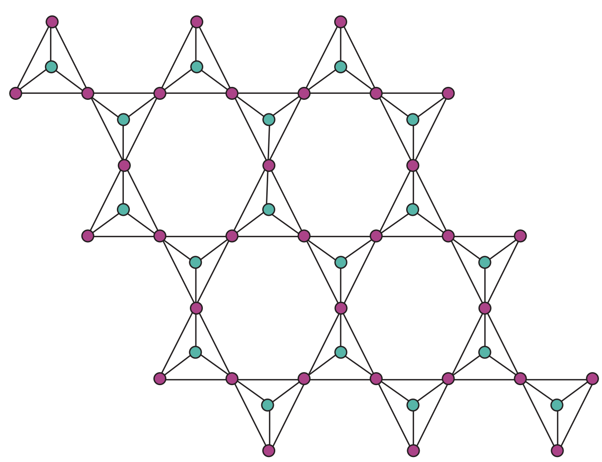

Figure 1: Rhombus silicate RHSL(3).

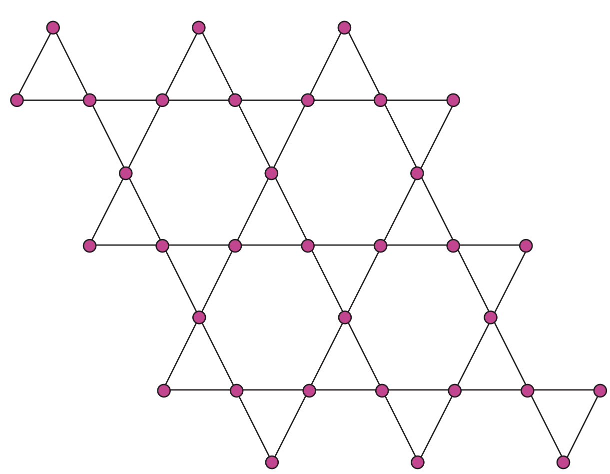

Figure 2: Rhombus oxide RHOX(3).

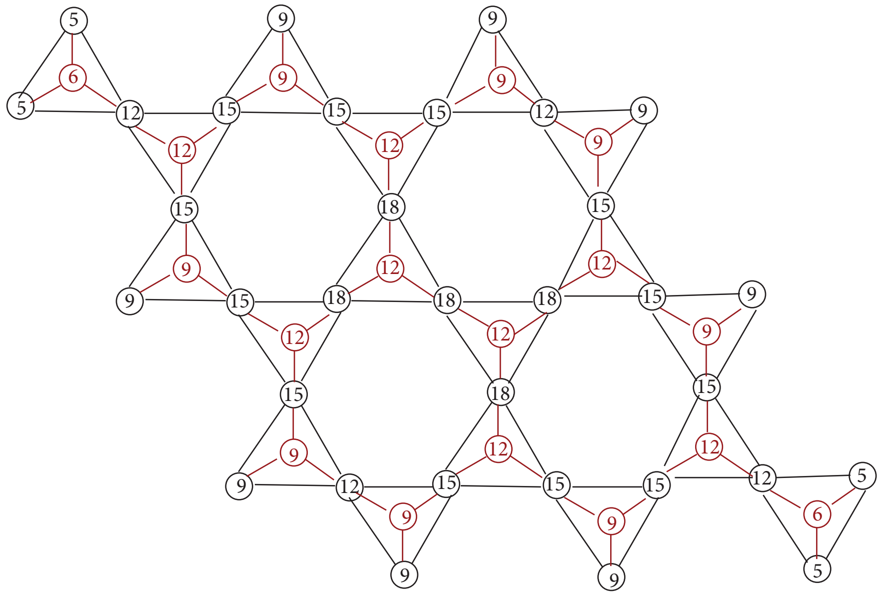

Figure 3: RHSL(3) along with CNs 5, 9, 12, 15, and 18.

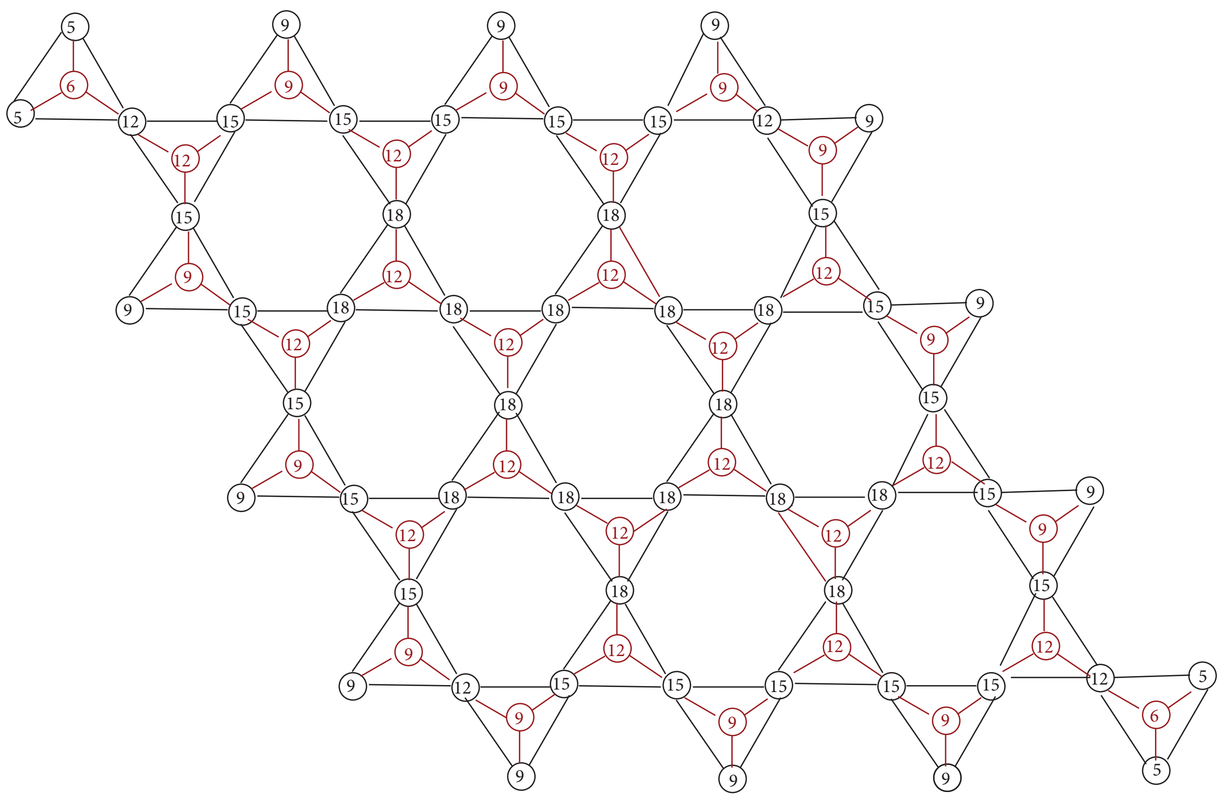

Figure 4: RHSL(4) along with CNs 5, 9, 12, 15, and 18.

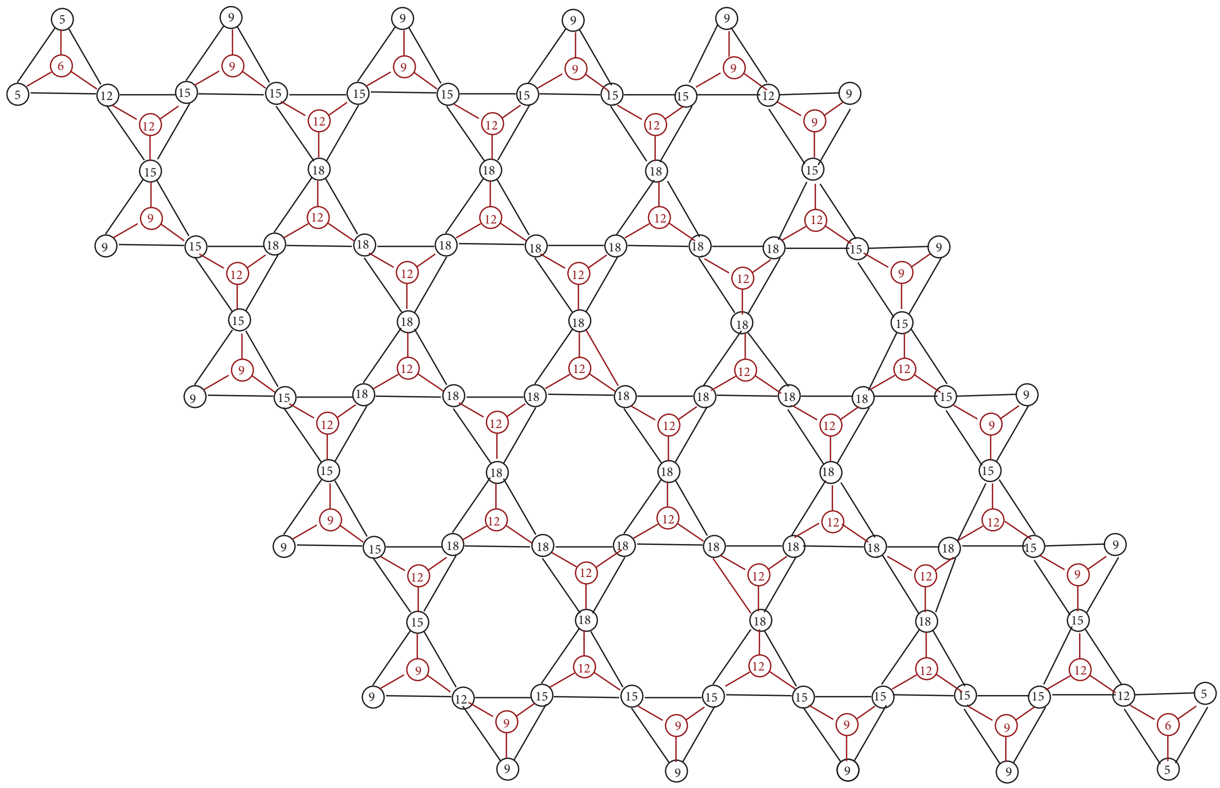

Figure 5: RHSL(5) along with CNs 5, 9, 12, 15, and 18.

By simple observation, one can see that there are a total of thirteen partitions of the edges. Thus, we have

$$\begin{aligned}
\mathcal{Q}_{(5,5)} &= \{tk \in \mathcal{Q}(\Upsilon)\colon \alpha(t) = 5, \alpha(k) = 5\},\\
\mathcal{Q}_{(5,6)} &= \{tk \in \mathcal{Q}(\Upsilon)\colon \alpha(t) = 5, \alpha(k) = 6\},\\
\mathcal{Q}_{(5,12)} &= \{tk \in \mathcal{Q}(\Upsilon)\colon \alpha(t) = 5, \alpha(k) = 12\},\\
\mathcal{Q}_{(6,12)} &= \{tk \in \mathcal{Q}(\Upsilon)\colon \alpha(t) = 6, \alpha(k) = 12\},\\
\mathcal{Q}_{(9,9)} &= \{tk \in \mathcal{Q}(\Upsilon)\colon \alpha(t) = 9, \alpha(k) = 9\},\\
\mathcal{Q}_{(9,12)} &= \{tk \in \mathcal{Q}(\Upsilon)\colon \alpha(t) = 9, \alpha(k) = 12\},\\
\mathcal{Q}_{(9,15)} &= \{tk \in \mathcal{Q}(\Upsilon)\colon \alpha(t) = 9, \alpha(k) = 15\}, \qquad (1)\\
\mathcal{Q}_{(12,12)} &= \{tk \in \mathcal{Q}(\Upsilon)\colon \alpha(t) = 12, \alpha(k) = 12\},\\
\mathcal{Q}_{(12,15)} &= \{tk \in \mathcal{Q}(\Upsilon)\colon \alpha(t) = 12, \alpha(k) = 15\},\\
\mathcal{Q}_{(12,18)} &= \{tk \in \mathcal{Q}(\Upsilon)\colon \alpha(t) = 12, \alpha(k) = 18\},\\
\mathcal{Q}_{(15,15)} &= \{tk \in \mathcal{Q}(\Upsilon)\colon \alpha(t) = 15, \alpha(k) = 15\},\\
\mathcal{Q}_{(15,18)} &= \{tk \in \mathcal{Q}(\Upsilon)\colon \alpha(t) = 15, \alpha(k) = 18\},\\
\mathcal{Q}_{(18,18)} &= \{tk \in \mathcal{Q}(\Upsilon)\colon \alpha(t) = 18, \alpha(k) = 18\}.
\end{aligned}$$

Total counts of the above-classified vertices are given in Table 3.

Table 3: Count of CN-based classified vertices of Υ.

$\mathcal{Q}_{(t,k)}$	$\lvert\mathcal{Q}_{(t,k)}\rvert$
$\mathcal{Q}_{(5,5)}$	2
$\mathcal{Q}_{(5,6)}$	4
$\mathcal{Q}_{(5,12)}$	4
$\mathcal{Q}_{(6,12)}$	2
$\mathcal{Q}_{(9,9)}$	$4m-4$
$\mathcal{Q}_{(9,12)}$	8
$\mathcal{Q}_{(9,15)}$	$16m-24$
$\mathcal{Q}_{(12,12)}$	2
$\mathcal{Q}_{(12,15)}$	$8m-4$
$\mathcal{Q}_{(12,18)}$	$6m^2-20m+16$
$\mathcal{Q}_{(15,15)}$	$8m-14$
$\mathcal{Q}_{(15,18)}$	$8m-16$
$\mathcal{Q}_{(18,18)}$	$6m^2-24m+24$

Theorem 1. *Let $\Upsilon = RHSL(m)$ be a molecular graph. Then, the ABCCI Υ) is given as*

$$\mathrm{ABCCI}(\Upsilon) = 4.1036m^2 + 1.7761m + 0.6205. \qquad (2)$$

Proof. By using Table 2 and definition of ABCCI, we have

$$\begin{aligned}
\mathrm{ABCCI}(\Upsilon) &= \sum_{t,k\in\mathcal{Q}(\Upsilon)} \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} \\
&= \left|\mathcal{Q}_{(5,5)}\right| \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} + \left|\mathcal{Q}_{(5,6)}\right| \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} + \left|\mathcal{Q}_{(5,12)}\right| \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} \\
&\quad + \left|\mathcal{Q}_{(6,12)}\right| \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} + \left|\mathcal{Q}_{(9,9)}\right| \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} + \left|\mathcal{Q}_{(9,12)}\right| \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} \\
&\quad + \left|\mathcal{Q}_{(9,15)}\right| \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} + \left|\mathcal{Q}_{(12,12)}\right| \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} + \left|\mathcal{Q}_{(12,15)}\right| \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} \\
&\quad + \left|\mathcal{Q}_{(12,18)}\right| \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} + \left|\mathcal{Q}_{(15,15)}\right| \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} + \left|\mathcal{Q}_{(15,18)}\right| \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} \\
&= \left|\mathcal{Q}_{(5,5)}\right| \sqrt{\frac{5+5-2}{5\times 5}} + \left|\mathcal{Q}_{(5,6)}\right| \sqrt{\frac{5+6-2}{5\times 6}} + \left|\mathcal{Q}_{(5,12)}\right| \sqrt{\frac{5+12-2}{5\times 12}} + \left|\mathcal{Q}_{(6,12)}\right| \sqrt{\frac{6+12-2}{6\times 12}} \\
&\quad + \left|\mathcal{Q}_{(9,9)}\right| \sqrt{\frac{9+9-2}{9\times 9}} + \left|\mathcal{Q}_{(9,12)}\right| \sqrt{\frac{9+12-2}{9\times 12}} + \left|\mathcal{Q}_{(9,15)}\right| \sqrt{\frac{9+15-2}{9\times 15}} + \left|\mathcal{Q}_{(12,12)}\right| \sqrt{\frac{12+12-2}{12\times 12}} \\
&\quad + \left|\mathcal{Q}_{(12,15)}\right| \sqrt{\frac{12+15-2}{12\times 15}} + \left|\mathcal{Q}_{(12,18)}\right| \sqrt{\frac{12+18-2}{12\times 18}} + \left|\mathcal{Q}_{(15,15)}\right| \sqrt{\frac{15+15-2}{15\times 15}} \\
&\quad + \left|\mathcal{Q}_{(15,18)}\right| \sqrt{\frac{15+18-2}{15\times 18}} + \left|\mathcal{Q}_{(18,18)}\right| \sqrt{\frac{18+18-2}{18\times 18}} \\
&= 10.402 + (1.7776\,\mathrm{m} - 1.7776) + (6.4590\,\mathrm{m} - 9.6885) + (2.9808\,\mathrm{m} - 1.4904) \\
&\quad + \left(2.1602m^2 - 7.200m + 5.7600\right) + (2.8216m - 4.9378) + (2.7107m - 5.4208) \\
&\quad + \left(1.9434m^2 - 7.7736m + 7.7736\right) \\
&= 4.1036m^2 + 1.7761m + 0.6205.
\end{aligned} \tag{3}$$

□

Theorem 2. *Let $\Upsilon = RHSL(m)$ be a molecular graph. Then, GACI is given as*

$$GACI(\Upsilon) = 37.8782m^2 - 16.5584m - 25.3876. \tag{4}$$

Proof. By using the definition of GACI, we have

$$\begin{aligned}
\mathrm{GACI}(\Upsilon) &= \sum_{t,k\in\mathcal{Q}(\Upsilon)} \frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)} \\
&= \left|\mathcal{Q}_{(5,5)}\right| \frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)} + \left|\mathcal{Q}_{(5,6)}\right| \frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)} + \left|\mathcal{Q}_{(5,12)}\right| \frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)} \\
&\quad + \left|\mathcal{Q}_{(6,12)}\right| \frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)} + \left|\mathcal{Q}_{(9,9)}\right| \frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)} + \left|\mathcal{Q}_{(9,12)}\right| \frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}
\end{aligned}$$

$$+\left|\mathcal{Q}_{(9,15)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}+\left|\mathcal{Q}_{(12,12)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}+\left|\mathcal{Q}_{(12,15)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}$$
$$+\left|\mathcal{Q}_{(12,18)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}+\left|\mathcal{Q}_{(15,15)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}+\left|\mathcal{Q}_{(15,18)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}$$
$$+\left|\mathcal{Q}_{(18,18)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}$$
$$=2\frac{2\sqrt{5\times 5}}{5+5}+4\frac{2\sqrt{5\times 6}}{5+6}+4\frac{2\sqrt{5\times 12}}{5+12}+2\frac{2\sqrt{6\times 12}}{6+12}+(4m-4)\frac{2\sqrt{9\times 9}}{9+9}$$
$$+8\frac{2\sqrt{9\times 12}}{9+12}+(16m-24)\frac{2\sqrt{9\times 15}}{9+15}+2\frac{2\sqrt{12\times 12}}{12+12}+(8m-4)\frac{2\sqrt{12\times 15}}{12+15}$$
$$+\left(6m^2-20m+16\right)\frac{2\sqrt{12\times 18}}{12+18}+(8m-14)\frac{2\sqrt{15\times 15}}{15+15}+(8m-16)\frac{2\sqrt{15\times 18}}{15+18}$$
$$+\left(6m^2-24m+24\right)\frac{2\sqrt{18\times 18}}{18+18}$$
$$=37.8782m^2-16.5584m-25.3876. \quad (5)$$

□

Theorem 3. *Let $\Upsilon = RHSL(m)$ be a molecular graph. Then, AZCI is given as*

$$AZCI(\Upsilon)=7431.64m^2-11205.83m+3635.91. \quad (6)$$

Proof. By using the definition of AZCI, we have

$$\mathrm{AZCI}(\Upsilon)=\sum_{t,k\in\mathcal{Q}(\Upsilon)}\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3$$
$$=\left|\mathcal{Q}_{(5,5)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3+\left|\mathcal{Q}_{(5,6)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3+\left|\mathcal{Q}_{(5,12)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3$$
$$+\left|\mathcal{Q}_{(6,12)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3+\left|\mathcal{Q}_{(9,9)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3+\left|\mathcal{Q}_{(9,12)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3$$
$$+\left|\mathcal{Q}_{(9,15)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3+\left|\mathcal{Q}_{(12,12)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3+\left|\mathcal{Q}_{(12,15)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3$$
$$+\left|\mathcal{Q}_{(12,18)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3+\left|\mathcal{Q}_{(15,15)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3+\left|\mathcal{Q}_{(15,18)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3$$
$$+\left|\mathcal{Q}_{(18,18)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3$$
$$=2\left[\frac{5\times 5}{5+5-2}\right]^3+4\left[\frac{5\times 6}{5+6-2}\right]^3+4\left[\frac{5\times 12}{5+12-2}\right]^3+2\left[\frac{6\times 12}{6+12-2}\right]^3+(4m-4)\left[\frac{9\times 9}{9+9-2}\right]^3$$
$$+8\left[\frac{9\times 12}{9+12-2}\right]^3+(16m-24)\left[\frac{9\times 15}{9+15-2}\right]^3+2\left[\frac{12\times 12}{12+12-2}\right]^3+(8m-4)\left[\frac{12\times 15}{12+15-2}\right]^3$$

$$
\begin{aligned}
&+\left(6m^2-20m+16\right)\left[\frac{12\times 18}{12+18-2}\right]^3\\
&+(8m-14)\left[\frac{15\times 15}{15+15-2}\right]^3+(8m-16)\left[\frac{15\times 18}{15+18-2}\right]^3+\left(6m^2-24m+24\right)\left[\frac{18\times 18}{8+8-2}\right]^3\\
&=7431.64m^2-11205.83m+3635.91.
\end{aligned}
\tag{7}
$$

□

Theorem 4. *Let $\Upsilon = RHSL(m)$ be a molecular graph. Then, SDCI is given as*

$$
\mathrm{SDCI}(\Upsilon)=25.0002m^2-2.0006m-9. \tag{8}
$$

Proof. By using the definition of SDCI, we have

$$
\begin{aligned}
\mathrm{SDCI}(\Upsilon) &= \sum_{t,k\in\mathcal{Q}(\Upsilon)}\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]\\
&=\left|\mathcal{Q}_{(5,5)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]+\left|\mathcal{Q}_{(5,6)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]\\
&+\left|\mathcal{Q}_{(5,12)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]+\left|\mathcal{Q}_{(6,12)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]\\
&+\left|\mathcal{Q}_{(9,9)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]+\left|\mathcal{Q}_{(9,12)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]\\
&+\left|\mathcal{Q}_{(9,15)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]+\left|\mathcal{Q}_{(12,12)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]\\
&+\left|\mathcal{Q}_{(12,15)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]+\left|\mathcal{Q}_{(12,18)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]\\
&+\left|\mathcal{Q}_{(15,15)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]+\left|\mathcal{Q}_{(15,18)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]\\
&+\left|\mathcal{Q}_{(18,18)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]\\
&=2\left[\frac{\min(5,5)}{\max(5,5)}+\frac{\max(5,5)}{\min(5,5)}\right]+4\left[\frac{\min(5,6)}{\max(5,6)}+\frac{\max(5,6)}{\min(5,6)}\right]+4\left[\frac{\min(5,12)}{\max(5,12)}+\frac{\max(5,12)}{\min(5,12)}\right]\\
&+2\left[\frac{\min(6,12)}{\max(6,12)}+\frac{\max(6,12)}{\min(6,12)}\right]+(4m-4)\left[\frac{\min(9,9)}{\max(9,9)}+\frac{\max(9,9)}{\min(9,9)}\right]\\
&+8\left[\frac{\min(9,12)}{\max(9,12)}+\frac{\max(9,12)}{\min(9,12)}\right]+(16m-24)\left[\frac{\min(9,15)}{\max(9,15)}+\frac{\max(9,15)}{\min(9,15)}\right]\\
&+2\left[\frac{\min(12,12)}{\max(12,12)}+\frac{\max(12,12)}{\min(12,12)}\right]+(8m-4)\left[\frac{\min(12,15)}{\max(12,15)}+\frac{\max(12,15)}{\min(12,15)}\right]\\
&+\left(6m^2-20m+16\right)\left[\frac{\min(12,18)}{\max(12,18)}+\frac{\max(12,18)}{\min(12,18)}\right]+(8m-14)\left[\frac{\min(15,15)}{\max(15,15)}+\frac{\max(15,15)}{\min(15,15)}\right]\\
&+(8m-16)\left[\frac{\min(15,18)}{\max(15,18)}+\frac{\max(15,18)}{\min(15,18)}\right]+\left(6m^2-24m+24\right)\left[\frac{\min(18,18)}{\max(18,18)}+\frac{\max(18,18)}{\min(18,18)}\right]\\
&=25.0002m^2-2.0006m-9.
\end{aligned}
\tag{9}
$$

□

Theorem 5. *Let $\Upsilon = RHSL(m)$ be a molecular graph. Then, HCI is given as*

$$HCI(\Upsilon) = 0.7332m^2 + 0.7212m + 0.50447. \quad (10)$$

Proof. By using the definition of HCI, we have

$$\begin{aligned}
HCI(\Upsilon) &= \sum_{t,k\in \mathcal{Q}(\Upsilon)} \frac{2}{(\alpha(t)+\alpha(k))}\\
&= |\mathcal{Q}_{(5,5)}|\frac{2}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(5,6)}|\frac{2}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(5,12)}|\frac{2}{(\alpha(t)+\alpha(k))}\\
&\quad + |\mathcal{Q}_{(6,12)}|\frac{2}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(9,9)}|\frac{2}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(9,12)}|\frac{2}{(\alpha(t)+\alpha(k))}\\
&\quad + |\mathcal{Q}_{(9,15)}|\frac{2}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(12,12)}|\frac{2}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(12,15)}|\frac{2}{(\alpha(t)+\alpha(k))}\\
&\quad + |\mathcal{Q}_{(12,18)}|\frac{2}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(15,15)}|\frac{2}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(15,18)}|\frac{2}{(\alpha(t)+\alpha(k))}\\
&\quad + |\mathcal{Q}_{(18,18)}|\frac{2}{(\alpha(t)+\alpha(k))}\\
&= 2\frac{2}{(5+5)} + 4\frac{2}{(5+6)} + 4\frac{2}{(5+12)} + 2\frac{2}{(6+12)} + (4m-4)\frac{2}{(9+9)}\\
&\quad + 8\frac{2}{(9+12)} + (16m-24)\frac{2}{(9+15)} + 2\frac{2}{(12+12)} + (8m-4)\frac{2}{(12+15)}\\
&\quad + \left(6m^2-20m+16\right)\frac{2}{(12+18)} + (8m-14)\frac{2}{(15+15)} + (8m-16)\frac{2}{(15+18)}\\
&\quad + \left(6m^2-24m+24\right)\frac{2}{(18+18)}\\
&= 0.7332m^2 + 0.7212m + 0.50447.
\end{aligned} \quad (11)$$

□

Theorem 6. *Let $\Upsilon = RHSL(m)$ be a molecular graph. Then, ISCI is given as*

$$\mathrm{ISCI}(\Upsilon) = 97.2m^2 + 2.6404m - 75.4745. \quad (12)$$

Proof. By using the definition of ISCI, we have

$$\begin{aligned}
\mathrm{ISCI}(\Upsilon) &= \sum_{t,k\in \mathcal{Q}(\Upsilon)} \frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))}\\
&= |\mathcal{Q}_{(5,5)}|\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(5,6)}|\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(5,12)}|\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))}\\
&\quad + |\mathcal{Q}_{(6,12)}|\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(9,9)}|\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(9,12)}|\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))}\\
&\quad + |\mathcal{Q}_{(9,15)}|\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(12,12)}|\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} + |\mathcal{Q}_{(12,15)}|\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))}
\end{aligned}$$

$$+\left|\mathcal{Q}_{(12,18)}\right|\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))}+\left|\mathcal{Q}_{(15,15)}\right|\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))}+\left|\mathcal{Q}_{(15,18)}\right|\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))}$$
$$+\left|\mathcal{Q}_{(18,18)}\right|\frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))}$$
$$=2\frac{5\times5}{(5+5)}+4\frac{5\times6}{(5+6)}+4\frac{5\times12}{(5+12)}+2\frac{6\times12}{(6+12)}+(4m-4)\frac{9\times9}{(9+9)}$$
$$+8\frac{9\times12}{(9+12)}+(16m-24)\frac{9\times15}{(9+15)}+2\frac{12\times12}{(12+12)}+(8m-4)\frac{12\times15}{(12+15)}$$
$$+\left(6m^2-20m+16\right)\frac{12\times18}{(12+18)}+(8m-14)\frac{15\times15}{(15+15)}+(8m-16)\frac{15\times18}{(15+18)}$$
$$+\left(6m^2-24m+24\right)\frac{18\times18}{(18+18)}$$
$$=97.2m^2+2.6404m-75.4745. \tag{13}$$

□

Theorem 7. *Let* $\Upsilon = RHSL(m)$ *be a molecular graph. Then, HZCI is given as*

$$HZCI(\Upsilon)=13176m^2-17820m+5584. \tag{14}$$

Proof. By using the definition of HZCI, we have

$$\begin{aligned}HZCI(\Upsilon)=&\sum_{t,k\in\mathcal{Q}(\Upsilon)}[\alpha(t)+\alpha(k)]^2\\
=&\left|\mathcal{Q}_{(5,5)}\right|[\alpha(t)+\alpha(k)]^2+\left|\mathcal{Q}_{(5,6)}\right|[\alpha(t)+\alpha(k)]^2+\left|\mathcal{Q}_{(5,12)}\right|[\alpha(t)+\alpha(k)]^2\\
&+\left|\mathcal{Q}_{(6,12)}\right|[\alpha(t)+\alpha(k)]^2+\left|\mathcal{Q}_{(9,9)}\right|[\alpha(t)+\alpha(k)]^2+\left|\mathcal{Q}_{(9,12)}\right|[\alpha(t)+\alpha(k)]^2\\
&+\left|\mathcal{Q}_{(9,15)}\right|[\alpha(t)+\alpha(k)]^2+\left|\mathcal{Q}_{(12,12)}\right|[\alpha(t)+\alpha(k)]^2+\left|\mathcal{Q}_{(12,15)}\right|[\alpha(t)+\alpha(k)]^2\\
&+\left|\mathcal{Q}_{(12,18)}\right|[\alpha(t)+\alpha(k)]^2+\left|\mathcal{Q}_{(15,15)}\right|[\alpha(t)+\alpha(k)]^2+\left|\mathcal{Q}_{(15,18)}\right|[\alpha(t)+\alpha(k)]^2\\
&+\left|\mathcal{Q}_{(18,18)}\right|[\alpha(t)+\alpha(k)]^2\\
=&2(5+5)^2+4(5+6)^2+4(5+12)^2+2(6+12)^2+(4m-4)(9+9)^2\\
&+8(9+12)^2+(16m-24)(9+15)^2+2(12+12)^2+(8m-4)(12+15)^2\\
&+\left(6m^2-20m+16\right)(12+18)^2+(8m-14)(15+15)^2+(8m-16)(15+18)^2\\
&+\left(6m^2-24m+24\right)(18+18)^2\\
=&13176m^2-17820m+5584.\end{aligned} \tag{15}$$

□

5. CN-Based ZIs of the RHOX Network

In this section, we calculate the CN-based ZIs of RHOX. Let $\Gamma = RHOX(m)$ be a molecular graph RHOX network, where $m \geq 2$ is the dimension of the network. In Figures 6–8, we represent the molecular graph of $\Gamma = (\mathcal{P}, \mathcal{Q})$ of $RHOX(m)$ for $m = 2, 3, 4$ by labeling the vertices with their CNs.

To find ZCIs of the RHOX network, we define the partitions of the edge set of Γ on the basis of CNs. By simple observation, one can see that there are a total of eight partitions of the edges. Thus, we have

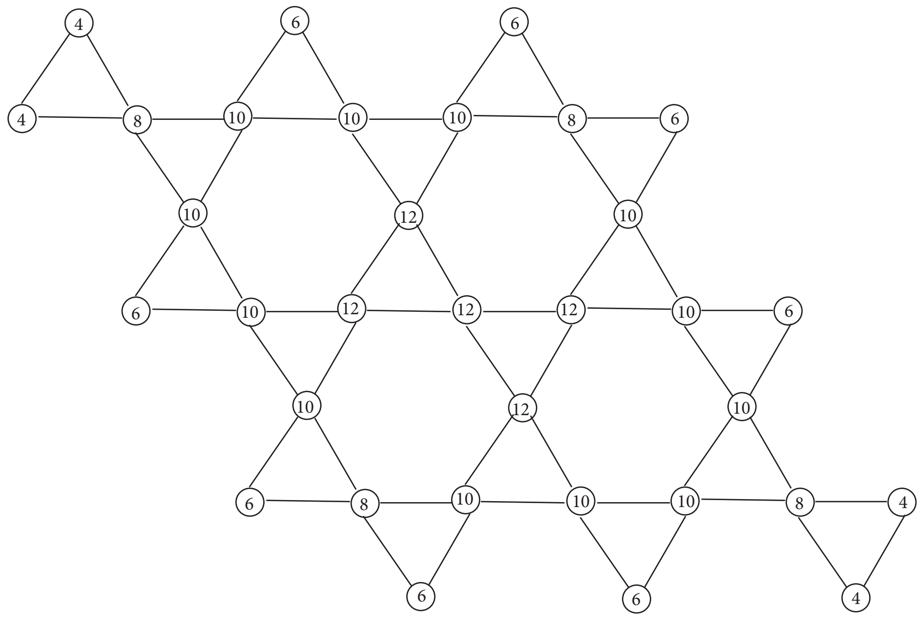

Figure 6: RHOX(3) along with CNs 4, 8, 6, 10, and 12.

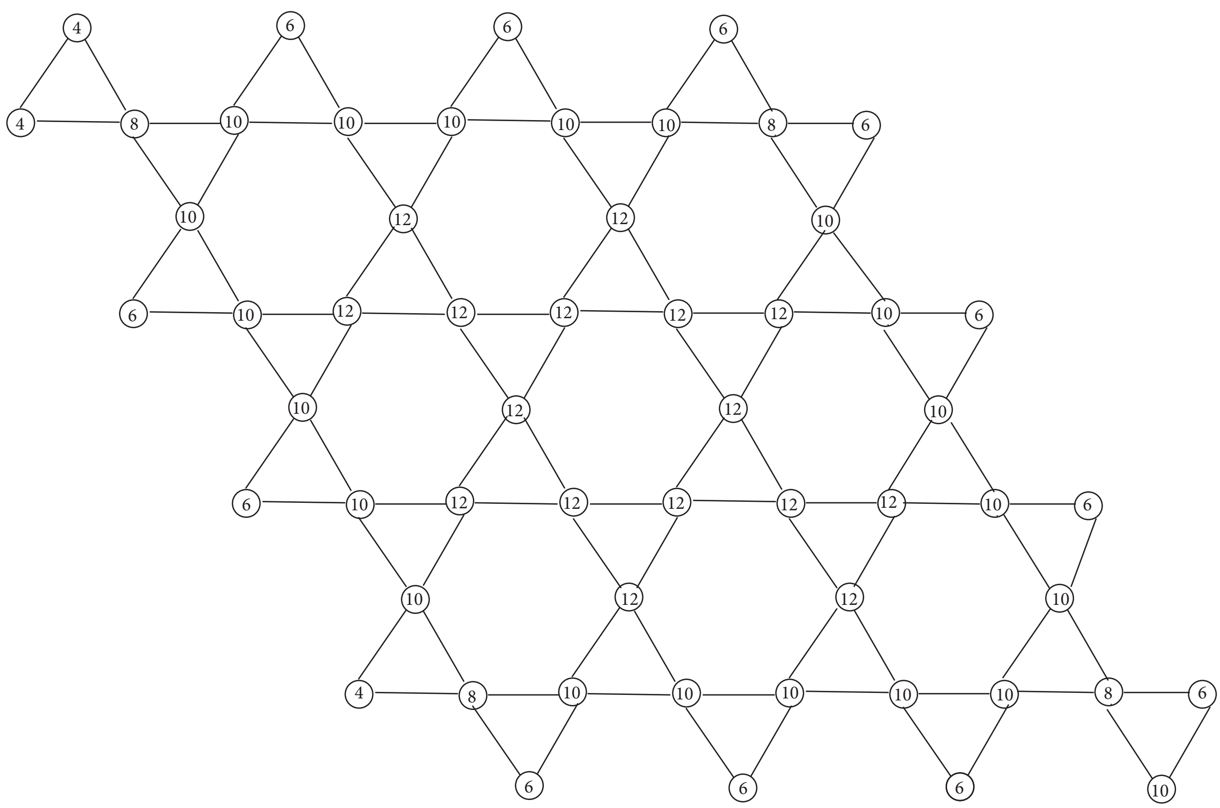

Figure 7: RHOX(4) along with CNs 4, 8, 6, 10, and 12.

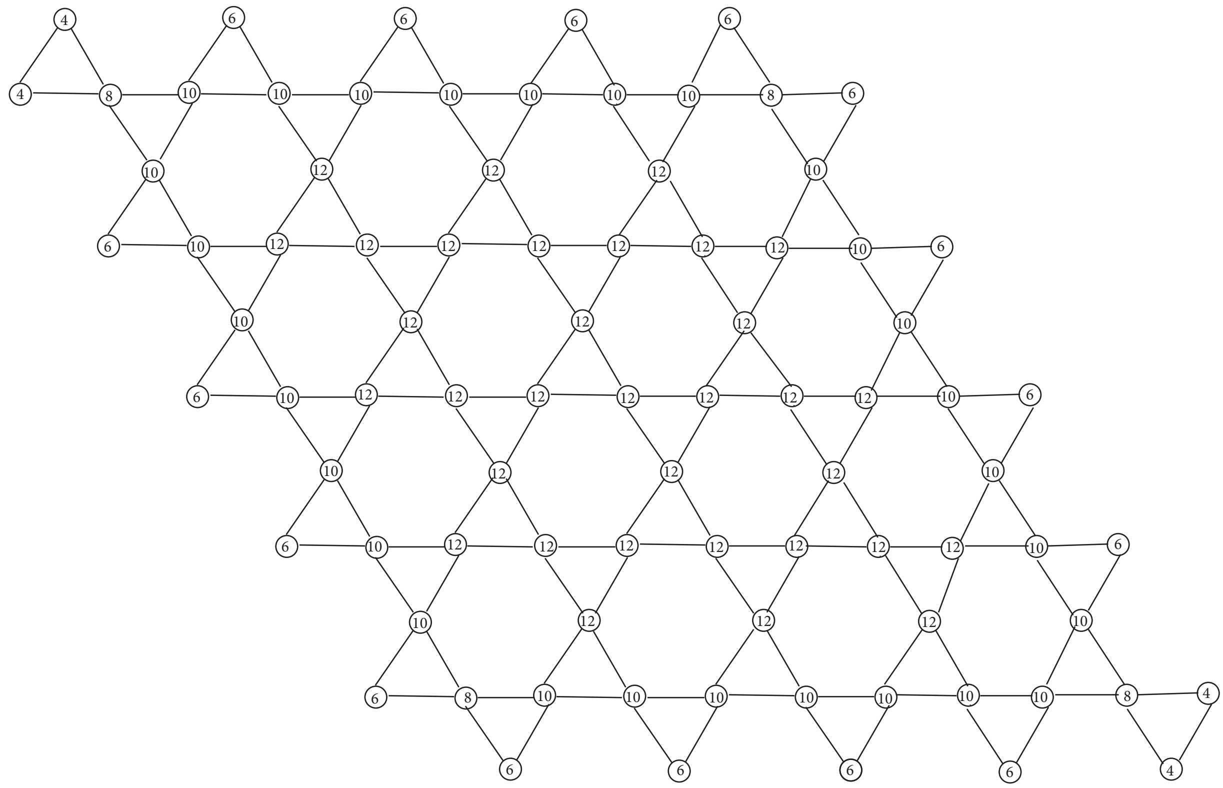

Figure 8: RHOX(5) along with CNs 4, 8, 6, 10, and 12.

$$
\begin{aligned}
\mathcal{Q}_{(4,4)} &= \{tk \in \mathcal{Q}(\Gamma)\colon \alpha(t) = 4, \alpha(k) = 4\},\\
\mathcal{Q}_{(4,8)} &= \{tk \in \mathcal{Q}(\Gamma)\colon \alpha(t) = 4, \alpha(k) = 8\}\\
\mathcal{Q}_{(6,8)} &= \{tk \in \mathcal{Q}(\Gamma)\colon \alpha(t) = 6, \alpha(k) = 8\},\\
\mathcal{Q}_{(6,10)} &= \{tk \in \mathcal{Q}(\Gamma)\colon \alpha(t) = 6, \alpha(k) = 10\}\\
\mathcal{Q}_{(8,10)} &= \{tk \in \mathcal{Q}(\Gamma)\colon \alpha(t) = 8, \alpha(k) = 10\},\\
\mathcal{Q}_{(10,10)} &= \{tk \in \mathcal{Q}(\Gamma)\colon \alpha(t) = 10, \alpha(k) = 10\},\\
\mathcal{Q}_{(10,12)} &= \{tk \in \mathcal{Q}(\Gamma)\colon \alpha(t) = 10, \alpha(k) = 12\},\\
\mathcal{Q}_{(12,12)} &= \{tk \in \mathcal{Q}(\Gamma)\colon \alpha(t) = 12, \alpha(k) = 12\}.
\end{aligned}
\tag{16}
$$

Total counts of the above-classified vertices are given in Table 4.

Table 4: Count of CN-based classified vertices of Γ.

$\mathcal{Q}_{(t,k)}$	$\lvert\mathcal{Q}_{(t,k)}\rvert$
$\mathcal{Q}_{(4,4)}$	2
$\mathcal{Q}_{(4,8)}$	4
$\mathcal{Q}_{(6,8)}$	4
$\mathcal{Q}_{(6,10)}$	$8m - 12$
$\mathcal{Q}_{(8,10)}$	8
$\mathcal{Q}_{(10,10)}$	$8m - 14$
$\mathcal{Q}_{(10,12)}$	$8m - 16$
$\mathcal{Q}_{(12,12)}$	$6m^2 - 24m + 24$

Theorem 8. *Let $\Gamma = RHOX(m)$ be a molecular graph. Then, ABCCI is given as*

$$
\mathrm{ABCCI}(\Gamma) = 2.3451m^2 - 2.2504m + 6.0899. \tag{17}
$$

Proof. By using the definition of ABCCI, we have

$$
\begin{aligned}
\mathrm{ABCCI}(\Gamma) &= \sum_{t,k\in\mathcal{Q}(\Gamma)} \sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}}\\
&= \left|\mathcal{Q}_{(4,4)}\right|\sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} + \left|\mathcal{Q}_{(4,8)}\right|\sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} + \left|\mathcal{Q}_{(6,8)}\right|\sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}}\\
&\quad + \left|\mathcal{Q}_{(6,10)}\right|\sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} + \left|\mathcal{Q}_{(8,10)}\right|\sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}} + \left|\mathcal{Q}_{(10,10)}\right|\sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}}
\end{aligned}
$$

$$+\left|\mathcal{Q}_{(10,12)}\right|\sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}}+\left|\mathcal{Q}_{(12,12)}\right|\sqrt{\frac{\alpha(t)+\alpha(k)-2}{\alpha(t)\times\alpha(k)}}$$

$$=\left|\mathcal{Q}_{(4,4)}\right|\sqrt{\frac{4+4-2}{4\times 4}}+\left|\mathcal{Q}_{(4,8)}\right|\sqrt{\frac{4+8-2}{4\times 8}}+\left|\mathcal{Q}_{(6,8)}\right|\sqrt{\frac{6+8-2}{6\times 8}}$$

$$+\left|\mathcal{Q}_{(6,10)}\right|\sqrt{\frac{6+10-2}{6\times 10}}+\left|\mathcal{Q}_{(8,10)}\right|\sqrt{\frac{8+10-2}{8\times 10}}+\left|\mathcal{Q}_{(10,10)}\right|\sqrt{\frac{10+10-2}{10\times 10}}$$

$$+\left|\mathcal{Q}_{(10,12)}\right|\sqrt{\frac{10+12-2}{10\times 12}}+\left|\mathcal{Q}_{(12,12)}\right|\sqrt{\frac{12+12-2}{12\times 12}}$$

$$= 2.3451m^2-2.2504m+6.0899. \tag{18}$$

□

Theorem 9. *Let Γ = RHOX (m) be a molecular graph. Then, GACI is given as*

$$GACI(\Gamma)=6m^2-0.288m-3.8459. \tag{19}$$

Proof. By using the definition of GACI, we have

$$\mathrm{GACI}(\Gamma)=\sum_{t,k\in\mathcal{Q}(\Gamma)}\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}$$

$$=\left|\mathcal{Q}_{(4,4)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}+\left|\mathcal{Q}_{(4,8)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}+\left|\mathcal{Q}_{(6,8)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}$$

$$+\left|\mathcal{Q}_{(6,10)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}+\left|\mathcal{Q}_{(8,10)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}+\left|\mathcal{Q}_{(10,10)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}$$

$$+\left|\mathcal{Q}_{(10,12)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)}+\left|\mathcal{Q}_{(12,12)}\right|\frac{2\sqrt{\alpha(t)\alpha(k)}}{\alpha(t)+\alpha(k)} \tag{20}$$

$$=2\frac{2\sqrt{4\times 4}}{4+4}+4\frac{2\sqrt{4\times 8}}{4+8}+4\frac{2\sqrt{6\times 8}}{6+8}+(8m-12)\frac{2\sqrt{6\times 10}}{6+10}+(8)\frac{2\sqrt{8\times 10}}{8+10}$$

$$+(8m-14)\frac{2\sqrt{10\times 10}}{10+10}+(8m-16)\frac{2\sqrt{10\times 12}}{10+12}+\left(6m^2-24m+24\right)\frac{2\sqrt{12\times 12}}{12+12}$$

$$=6m^2-0.288m-3.8459.$$

□

Theorem 10. *Let Γ = RHOX (m) be a molecular graph. Then, AZCI is given as*

$$AZCI(\Gamma)=1682.52m^2-3000.7m+1353.94. \tag{21}$$

Proof. By using the definition of AZCI, we have

$$\mathrm{AZCI}(\Gamma)=\sum_{t,k\in\mathcal{Q}(\Gamma)}\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3$$

$$=\left|\mathcal{Q}_{(4,4)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3+\left|\mathcal{Q}_{(4,8)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3+\left|\mathcal{Q}_{(6,8)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3$$

$$+\left|\mathcal{Q}_{(6,10)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3+\left|\mathcal{Q}_{(8,10)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3+\left|\mathcal{Q}_{(10,10)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3$$
$$+\left|\mathcal{Q}_{(10,12)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3+\left|\mathcal{Q}_{(12,12)}\right|\left[\frac{\alpha(t)\times\alpha(k)}{\alpha(t)+\alpha(k)-2}\right]^3$$
$$=2\left[\frac{4\times4}{4+4-2}\right]^3+4\left[\frac{4\times8}{4+8-2}\right]^3+4\left[\frac{6\times8}{6+8-2}\right]^3+(8m-12)\left[\frac{6\times10}{6+10-2}\right]^3$$
$$+8\left[\frac{8\times10}{8+10-2}\right]^3+(8m-14)\left[\frac{10\times10}{10+10-2}\right]^3+(8m-16)\left[\frac{10\times12}{10+12-2}\right]^3$$
$$+\left(6m^2-24m+24\right)\left[\frac{12\times12}{12+12-2}\right]^3$$
$$=1682.52m^2-3000.7m+1353.94. \tag{22}$$

□

Theorem 11. *Let $\Gamma = RHOX(m)$ be a molecular graph. Then, SDCI is given as*

$$SDCI(\Gamma)=12m^2+2.3988m-2.999. \tag{23}$$

Proof. By using the definition of SDCI, we have

$$\mathrm{SDCI}(\Gamma)=\sum_{t,k\in\mathcal{Q}(\Gamma)}\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]$$
$$=\left|\mathcal{Q}_{(4,4)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]+\left|\mathcal{Q}_{(4,8)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]$$
$$+\left|\mathcal{Q}_{(6,8)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]+\left|\mathcal{Q}_{(6,10)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]$$
$$+\left|\mathcal{Q}_{(8,10)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]+\left|\mathcal{Q}_{(10,10)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]$$
$$+\left|\mathcal{Q}_{(10,12)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right]+\left|\mathcal{Q}_{(12,12)}\right|\left[\frac{\min(\alpha(t),\alpha(k))}{\max(\alpha(t),\alpha(k))}+\frac{\max(\alpha(t),\alpha(k))}{\min(\alpha(t),\alpha(k))}\right] \tag{24}$$
$$=2\left[\frac{\min(4,4)}{\max(4,4)}+\frac{\max(4,4)}{\min(4,4)}\right]+4\left[\frac{\min(4,8)}{\max(4,8)}+\frac{\max(4,8)}{\min(4,8)}\right]+4\left[\frac{\min(6,8)}{\max(6,8)}+\frac{\max(6,8)}{\min(6,8)}\right]$$
$$+(8m-12)\left[\frac{\min(6,10)}{\max(6,10)}+\frac{\max(6,10)}{\min(6,10)}\right]+8\left[\frac{\min(8,10)}{\max(8,10)}+\frac{\max(8,10)}{\min(8,10)}\right]$$
$$+(8m-14)\left[\frac{\min(10,10)}{\max(10,10)}+\frac{\max(10,10)}{\min(10,10)}\right]+(8m-16)\left[\frac{\min(10,12)}{\max(10,12)}+\frac{\max(10,12)}{\min(10,12)}\right]$$
$$+\left(6m^2-24m+24\right)\left[\frac{\min(12,12)}{\max(12,12)}+\frac{\max(12,12)}{\min(12,12)}\right]$$
$$=12m^2+2.3988m-2.999.$$

□

Theorem 12. *Let* $\Gamma = RHOX(m)$ *be a molecular graph. Then, HCI is given as*

$$\mathrm{HCI}(\Gamma) = 0.5m^2 + 0.52728m + 1.377244. \quad (25)$$

Proof. By using the definition of HCI, we have

$$\begin{aligned}
\mathrm{HCI}(\Gamma) &= \sum_{t,k\in \mathcal{Q}(\Gamma)} \frac{2}{(\alpha(t)+\alpha(k))} \\
&= \left|\mathcal{Q}_{(4,4)}\right| \frac{2}{(\alpha(t)+\alpha(k))} + \left|\mathcal{Q}_{(4,8)}\right| \frac{2}{(\alpha(t)+\alpha(k))} + \left|\mathcal{Q}_{(6,8)}\right| \frac{2}{(\alpha(t)+\alpha(k))} \\
&\quad + \left|\mathcal{Q}_{(6,10)}\right| \frac{2}{(\alpha(t)+\alpha(k))} + \left|\mathcal{Q}_{(8,10)}\right| \frac{2}{(\alpha(t)+\alpha(k))} + \left|\mathcal{Q}_{(10,10)}\right| \frac{2}{(\alpha(t)+\alpha(k))} \\
&\quad + \left|\mathcal{Q}_{(10,12)}\right| \frac{2}{(\alpha(t)+\alpha(k))} + \left|\mathcal{Q}_{(12,12)}\right| \frac{2}{(\alpha(t)+\alpha(k))} \\
&= 2\frac{2}{(4+4)} + 4\frac{2}{(4+8)} + 4\frac{2}{(6+8)} + (8m-12)\frac{2}{(6+10)} + 8\frac{2}{(8+10)} \\
&\quad + (8m-14)\frac{2}{(10+10)} + (8m-16)\frac{2}{(10+12)} + \left(6m^2-24m+24\right)\frac{2}{(12+12)} \\
&= 0.5m^2 + 0.52728m + 1.377244.
\end{aligned} \quad (26)$$

□

Theorem 13. *Let* $\Gamma = RHOX(m)$ *be a molecular graph. Then, ISCI is given as*

$$ISCI(\Gamma) = 36m^2 - 30.364m + 5.663. \quad (27)$$

Proof. By using the definition of ISCI, we have

$$\begin{aligned}
\mathrm{ISCI}(\Gamma) &= \sum_{t,k\in \mathcal{Q}(\Gamma)} \frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} \\
&= \left|\mathcal{Q}_{(4,4)}\right| \frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} + \left|\mathcal{Q}_{(4,8)}\right| \frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} + \left|\mathcal{Q}_{(6,8)}\right| \frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} \\
&\quad + \left|\mathcal{Q}_{(6,10)}\right| \frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} + \left|\mathcal{Q}_{(8,10)}\right| \frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} + \left|\mathcal{Q}_{(10,10)}\right| \frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} \\
&\quad + \left|\mathcal{Q}_{(10,12)}\right| \frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} + \left|\mathcal{Q}_{(12,12)}\right| \frac{\alpha(t)\times\alpha(k)}{(\alpha(t)+\alpha(k))} \\
&= 2\frac{4\times4}{(4+4)} + 4\frac{4\times8}{(4+8)} + 4\frac{6\times8}{(6+8)} + (8m-12)\frac{6\times10}{(6+10)} + 8\frac{8\times10}{(8+10)} \\
&\quad + (8m-14)\frac{10\times10}{(10+10)} + (8m-16)\frac{10\times12}{(10+12)} + \left(6m^2-24m+24\right)\frac{12\times12}{(12+12)} \\
&= 36m^2 - 30.364m + 5.663.
\end{aligned} \quad (28)$$

□

Table 5: Computed values of CBZIs of RHSL for $m = 2, 3, \ldots, 8$.

CBZIs	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$	$m = 7$	$m = 8$
ABCCI (ϒ)	20.5871	42.8812	73.3825	112.091	159.0067	214.1296	277.4597
GACI (ϒ)	93.0084	265.841	514.43	838.7754	1238.8772	1714.7354	2266.35
AZCI (ϒ)	10950.81	36903.18	77718.83	133397.76	203939.97	289345.46	389614.23
SDCI (ϒ)	86.9996	210	383.0008	606.002	879.0036	1202.0056	1575.008
HCI (ϒ)	4.87967	9.26687	15.12047	22.44047	31.22687	41.47967	53.19887
ISCI (ϒ)	318.6063	807.2467	1490.2871	2367.7275	3439.5679	4705.8083	6166.4487
HZCI (ϒ)	22648	70708	145120	245884	373000	526468	706288

Table 6: Computed values CBZIs for $m = 2, 3, \ldots, 8$.

CBZIs	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$	$m = 7$	$m = 8$
$ABCCI\,(\Gamma)$	15.469	27.1955	43.61130	64.71724	90.51336	120.99	156.176
$GACI\,(\Gamma)$	19.5781	49.2901	91.0021	144.7141	210.4261	288.1381	377.8501
$AZCI\,(\Gamma)$	2082.62	7494.52	16271.46	28413.44	43920.46	62792.52	85029.62
$SDCI\,(\Gamma)$	49.798	112.19	198.59	308.995	443.3938	601.792	784.191
$HCI\,(\Gamma)$	4.4318	7.4590	11.486	16.51364	22.54092	29.5682	37.595
$ISCI\Gamma$	88.935	238.57	460.20	753.84	1119.4	1557.1	2066.7
$HZCI\,(\Gamma)$	5904	18480	37928	64368	97680	137904	185040

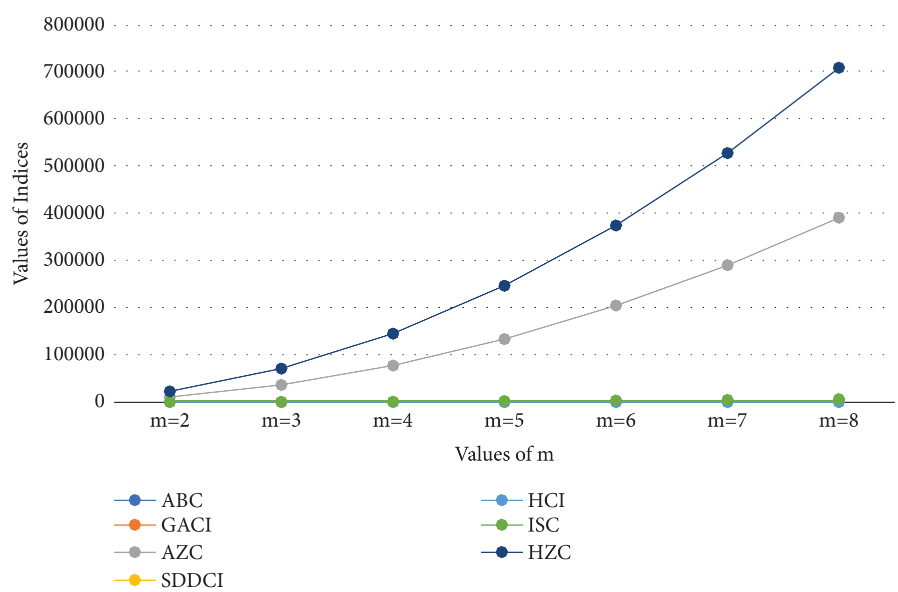

Figure 9: Comparison of TIs of the rhombus silicate network.

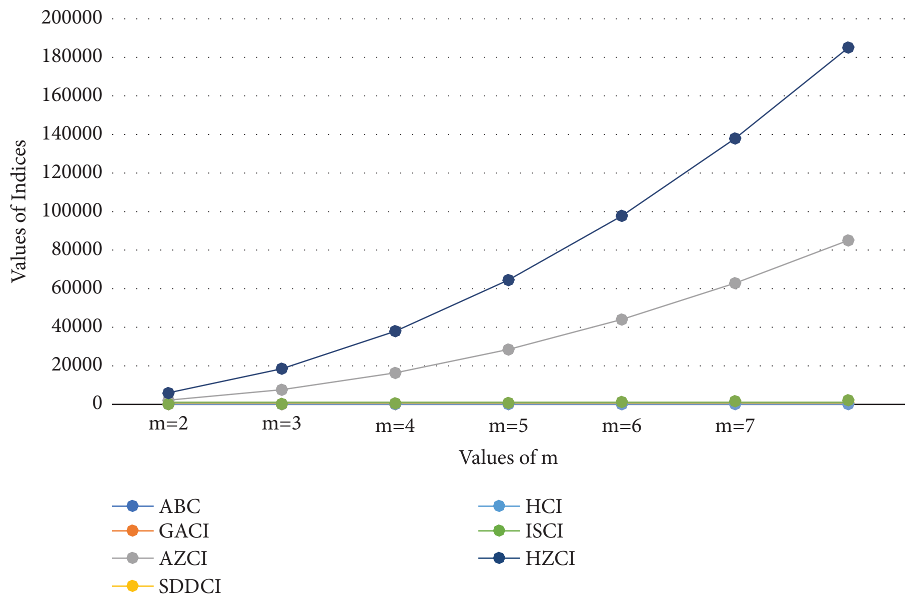

Figure 10: Comparison of TIs of the rhombus oxide network.

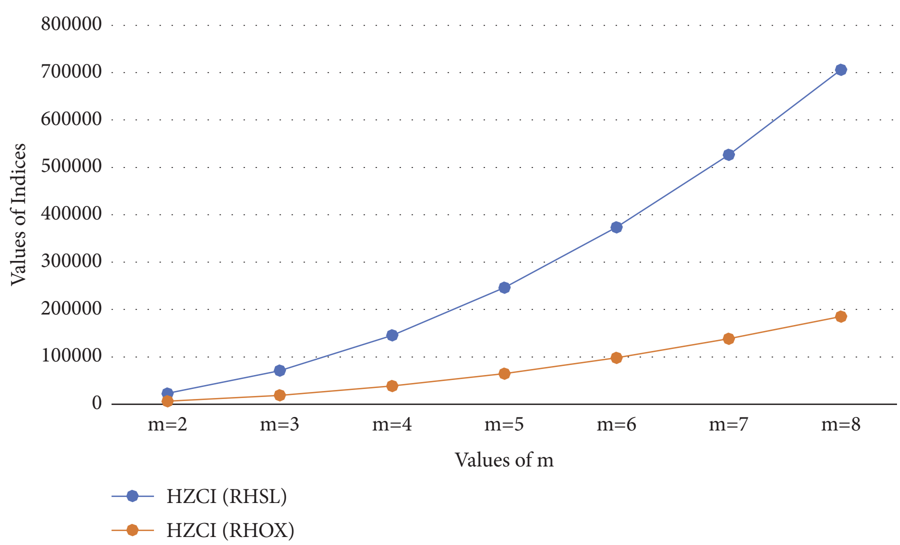

Figure 11: Comparison of RHSL and RHOX networks.

Table 7: Computed values of ZIs for RHSL for $m = 2, 3, \ldots, 8$.

CBZIs	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$	$m = 7$	$m = 8$
ABCI(RHSL)	29.612	65.0762	114.3482	177.428	254.3156	345.011	449.5142
GAI(RHSL)	46.3985	104.4538	185.8227	290.5052	418.5013	569.811	744.4343
AZI(RHSL)	1055.9472	2705.7402	5119.44	8297.0466	12238.56	16943.9802	22413.3072

Table 8: Computed values of ZIs for RHOX for $m = 2, 3, \ldots, 8$.

CBZIs	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$	$m = 7$	$m = 8$
ABCI(RHOX)	16.023	35.151	61.629	95.4546	136.6286	185.151	241.0218
GAI(RHOX)	23.3137	52.8562	94.3987	147.9412	213.4837	291.0262	380.5687
AZI(RHOX)	301.5994	782.7462	1491.433	2427.6598	3591.4266	4982.7334	6601.5802

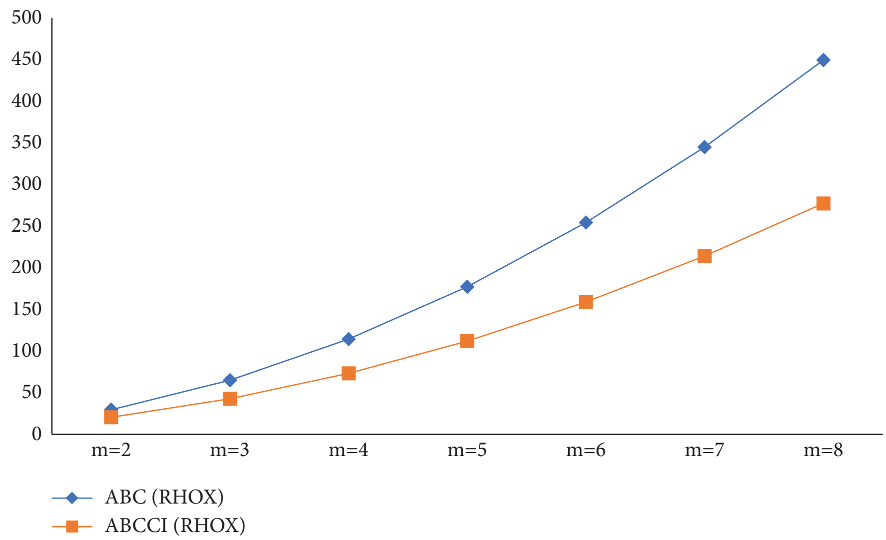

Figure 12: Graphical comparison of ABCI and ABCCI for the RHSL network.

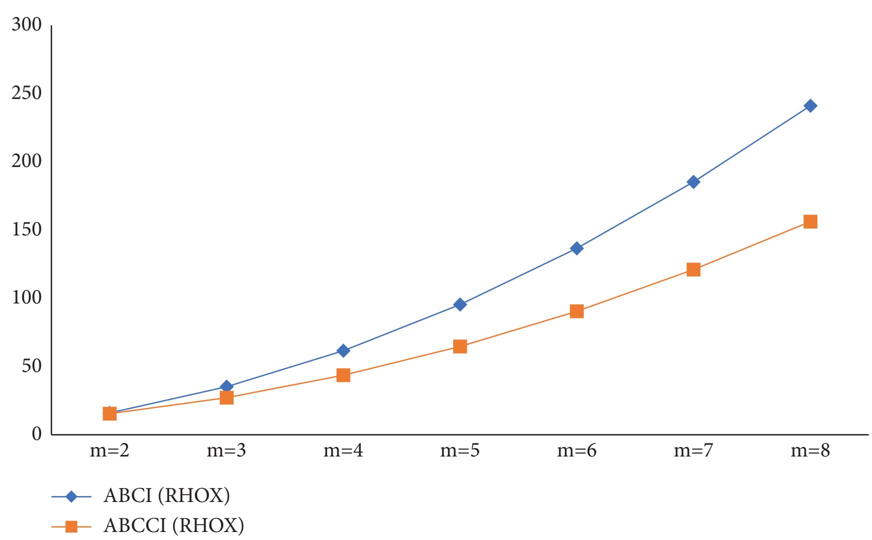

Figure 13: Graphical comparison of ABCI and ABCCI for the RHOX network.

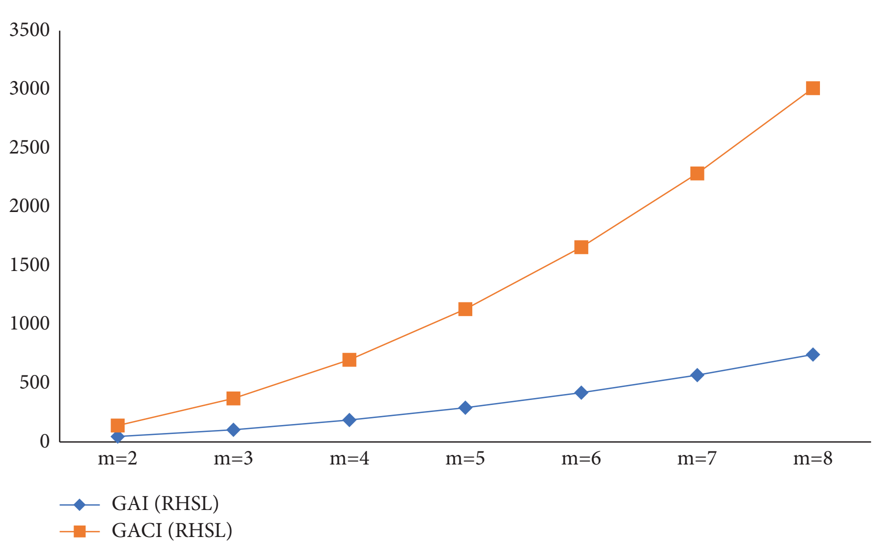

Figure 14: Graphical comparison of GAI and GACI for the RHSL network.

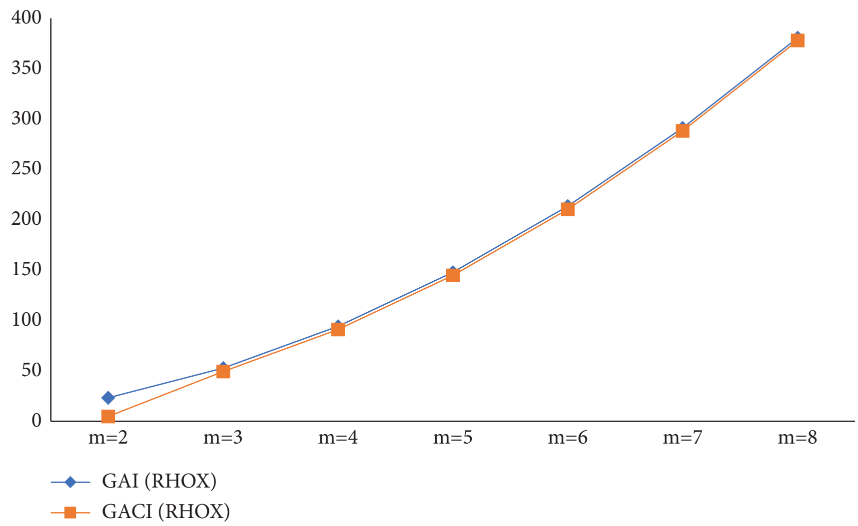

FIGURE 15: Graphical comparison of GAI and GACI for the RHOX network.

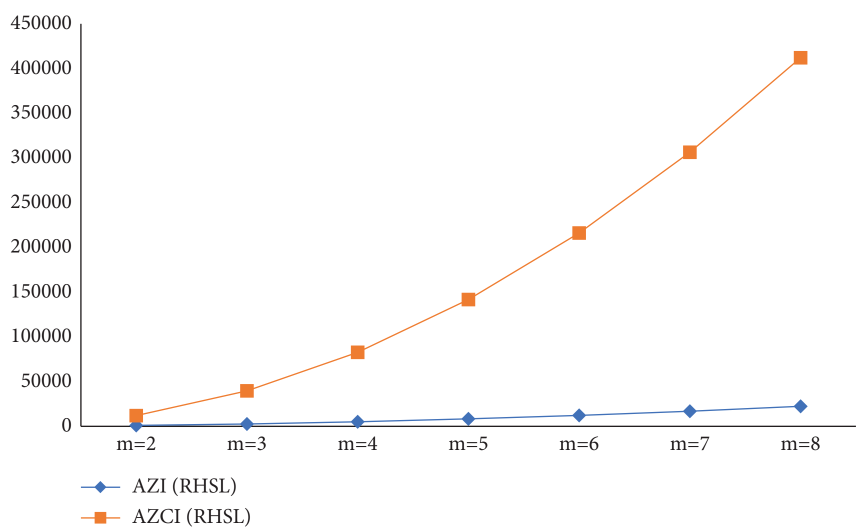

FIGURE 16: Graphical comparison of AZI and AZCI for the RHSL network.

Theorem 14. *Let $\Gamma = RHOX(m)$ be a molecular graph. Then, HZCI is given as*

$$HZCI(\Gamma) = 3456m^2 - 4704m + 1488. \tag{29}$$

Proof. By using the definition of HZCI, we have

$$\begin{aligned}
\mathrm{HZCI}(\Gamma) &= \sum_{t,k\in\mathcal{Q}(\Gamma)} [\alpha(t)+\alpha(k)]^2,\\
&= \left|\mathcal{Q}_{(4,4)}\right|[\alpha(t)+\alpha(k)]^2 + \left|\mathcal{Q}_{(4,8)}\right|[\alpha(t)+\alpha(k)]^2 + \left|\mathcal{Q}_{(6,8)}\right|[\alpha(t)+\alpha(k)]^2\\
&\quad + \left|\mathcal{Q}_{(6,10)}\right|[\alpha(t)+\alpha(k)]^2 + \left|\mathcal{Q}_{(8,10)}\right|[\alpha(t)+\alpha(k)]^2 + \left|\mathcal{Q}_{(10,10)}\right|[\alpha(t)+\alpha(k)]^2\\
&\quad + \left|\mathcal{Q}_{(10,12)}\right|[\alpha(t)+\alpha(k)]^2 + \left|\mathcal{Q}_{(12,12)}\right|[\alpha(t)+\alpha(k)]^2\\
&= 2(4+4)^2 + 4(4+8)^2 + 4(6+8)^2 + (8m-12)(6+10)^2 + 8(8+10)^2\\
&\quad + (8m-14)(10+10)^2 + (8m-16)(10+12)^2 + \left(6m^2-24m+24\right)(12+12)^2\\
&= 3456m^2 - 4704m + 1488.
\end{aligned} \tag{30}$$

□

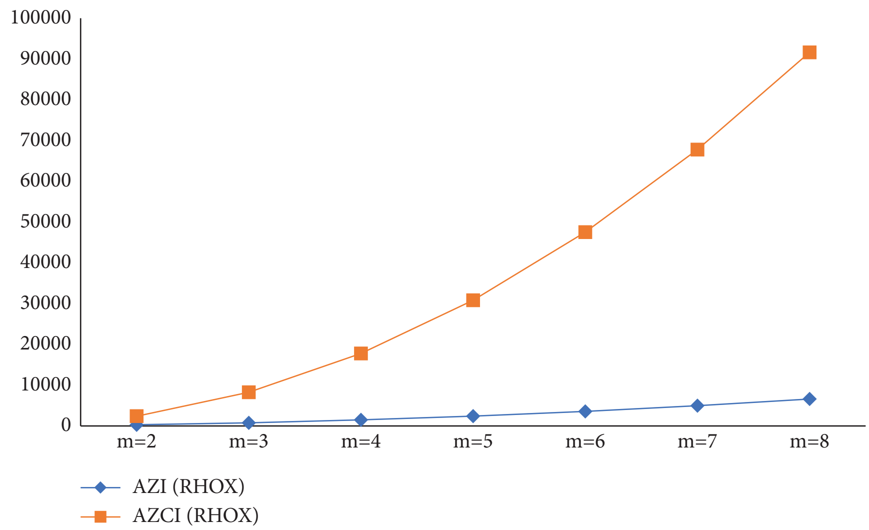

Figure 17: Graphical comparison of AZI and AZCI for the RHOX network.

6. Comparative Analysis

6.1. Comparison among Connection-Based TIs for RHSL and RHOX Networks. In this section, we individually compare the results of all the calculated CBZI for the rhombus silicate and rhombus oxide networks using line graphs. In Sections 3 and 4, we have computed the general results of RHSL and RHOX networks in terms of m where m is the dimension. In Tables 5 and 6, we have computed the values of CBZIs of RHSL and RHOX networks for $m = 2, 3 \cdots 8$, respectively. In Figure 9, we have taken the values of m along the horizontal axis and the computed values of the indices along the vertical axis. From Figure 9, it is clear that the computed values of all the indices other than AZCI and HZCI coincide. HZCI attains the higher values for the RHSL network. Similarly, in Figure 10, we can see that computed values of all the indices other than AZCI and HZCI coincide and HZCI attains the maximum value for the RHOX network.

From Figures 9 and 10, it can be seen that HZCI has the maximum value for RHSL and RHOX networks. In Figure 11, we compare RHSL and RHOX networks.

From Figure 11, it is clear that computed values of HZCI for the RHSL network show a clear difference with the increasing values of m than that of the RHOX network.

6.2. Comparison among Degree-Based and Connection-Based Indices for RHSL. In this section, we compare our computed CBZIs with some degree-based indices which were calculated by Javaid et al. [30] in 2017. The expressions to calculate degree-based indices of RHSL(m) are given as follows:

$$\begin{aligned} \mathrm{ABCI}(\mathrm{RHSL}) &= 6.9039m^2 + 0.9447m + 0.1070, \\ \mathrm{GAI}(\mathrm{RHSL}) &= 11.6568m^2 - 0.2287m + 0.2287, \\ \mathrm{AZI}(\mathrm{RHSL}) &= 381.9534m^2 - 259.674m + 48.0816. \end{aligned} \tag{31}$$

Expressions to calculate degree-based indices of RHOX(m) are given as follows:

$$\begin{aligned} \mathrm{ABCI}(\mathrm{RHOX}) &= 3.6742m^2 + 0.7578m - 0.1894, \\ \mathrm{GAI}(\mathrm{RHOX}) &= 6m^2 - 0.4575m + 0.2287, \\ \mathrm{AZI}(\mathrm{RHOX}) &= 113.7774m^2 - 87.7032m + 21.9258. \end{aligned} \tag{32}$$

Numerical values of connection-based indices for RHSL and RHOX networks are given in Tables 7 and 8.

The graphical comparison between degree-based and connection-based indices for both RHSL and RHOX networks is shown in Figures 12–17.

7. Conclusion

In this paper, we studied CN-based ZIs, namely, atom-bond connectivity connection index, geometric-arithmetic index, symmetric degree index, harmonic index, inverse sum index, and hyper-Zagreb index of RHSL and RHOX networks and developed the closed formulas of these structures. These developed TIs will help in comprehending the underlying topologies of these networks. Furthermore, we have compared computed connection-based indices with degree-based indices of the literature. Also, we have compared calculated TIs with each other for RHSL and RHOX networks and compared both networks with each other on the basis of our computed connection-based indices. In future, we compute Zagreb connection indices for the other types of chemical structures.

Data Availability

The data used to support the findings of this study are included within this article and are available from the corresponding author on request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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