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Research Article

Topological Aspects of Molecular Networks: Crystal Cubic Carbons

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Theory of networks serves as a mathematical foundation for the construction and modeling of chemical structures and complicated networks. In particular, chemical networking theory has a wide range of utilizations in the study of chemical structures, where examination and manipulation of chemical structural information are made feasible by utilizing the numerical graph invariants. A network invariant or a topological index (TI) is a numerical measure of a chemical compound which is capable to describe the chemical structural properties such as melting point, freezing point, density, pressure, tension, and temperature of chemical compounds. Wiener initiated the first distance-based TI which is considered to be the most important TI to preserve the chemical and physical properties of chemical structures. Later on, degree-based TI was introduced to find the π-electron energy of molecules. Recently, connection number-based TIs are studied which are more efficient than degree and distance-based TIs. In this paper, we compute the connection number-based TIs of the structure of crystal cubic carbons which are one of the most significant and interesting composites in modern resources of science due to the involvement of carbon atoms.

1. Introduction

Mathematical chemistry, the field of theoretical chemistry, utilizes the mathematical tools to explain and predict chemical structures and complicated networks. Chemical network theory (NT) is a field of mathematical chemistry in which we use methods of network theory to mathematically represent the chemical phenomena of molecular chemical structures. NT is used to describe, develop, analyze, and comprehend the molecular structures and their characteristics. In chemical NT, chemical structures are incorporated by vertices and edges, where the vertices (nodes) speak to the atoms while the edges speak to the bonds between the atoms. This theory plays an important function in the realm of chemical sciences.

Chemical NT uses network theoretic invariants to restrict the molecular structure into a unique number that reveals the electronic structures, structural sections, and energy of atoms. Interpreting the molecular structural information with the help of these TIs is gaining popularity among the researchers over the years. The research work in the area of chemical NT regarding the topological utilizations nanostructures, polyphenylene dendrimer nanostars, tree like polyphenylene, carbon nanocones, extremal pentagonal chains, spiro hexagonal systems, and polyomino chains can be seen in [1–3]. These chemical applications inspired us to investigate TIs of some novel chemical networks. A huge number of early medication studies indicate that substantial internal linkages exist between the pharmacology and biomedical properties of drugs and their subatomic compositions. The topological descriptors such as

Zagreb indices (ZIs) and modified ZIs were defined to be used in the investigation of medication subatomic structures, which are very helpful for medicinal and pharmaceutical research.

There are many chemical substances that are beneficial for the survival of living things. The basic components that help in the formation of cells in living beings are oxygen, nitrogen, hydrogen, and carbon. The essential component for the human life is carbon. It is important for the production of proteins, carbohydrates, and nucleic acids. It is also essential for plant development in the form of carbon dioxide. It is found in the form of carbonates and bicarbonates in oceans, as a good conductor of electricity, and in the form of limestone in rocks. The particles of carbon may connect in distinct ways, which are referred to as allotropes of carbon. Carbon atom is well recognized in the shape of diamond, graphite, bucky balls, etc. The structure of distinct carbon allotropes is represented in Figure 1. In the structure of crystal cubic carbon, the carbon atoms are piled tightly together which make it a very strong material. There are wide ranging utilizations of carbon allotropes (for details, we refer the readers to [4–6]).

The Wiener index initiated by Wiener in 1947 while researching the boiling point of paraffin was the fundamental TI [7]. Gutman [8] initiated degree-based TIs. Following that, researchers investigated a variety of distance-based descriptors in chemical fields which helped them to interpret the chemical molecular information of chemical structures such as freezing and melting point, flammability, stability, and density. For more information, see [9, 10].

Gutman and Trinajstic [11] examined the new notion of the first ZI in 1975. Gutman et al. [12] then pioneered the unique concept of second ZI in 1975. Due to the vast span of their applications, these classical ZIs are very important in the study of chemical NT. Later on, Furtula and Gutman [13] proposed the notion of third ZI, which is also known as the forgotten index since it was discovered after a lengthy period of time. Nikolic et al. [14] investigated modified ZI in 2003. In 2018, Yang et al. [15] found some degree-based ZIs of the crystal cubic carbon structures. Gao et al. [16] and Zahid et al. [17] computed the ZIs of crystal cubic carbon structures. Further, Zhang and Naeem [18] found the metric dimension of these structures of carbon atom. Moreover, Yang et al. [19] computed the vertex Szeged index of the structure of cubic crystals. Furthermore, Arockiaraj et al. [20] and Abraham et al. [21] explored the topological properties of other types of three-dimensional structures. Recently, Ali and Trinajstić [22] initiated a novel conception of connection number (CN) which is the cardinality of those nodes having length two from a certain vertex. They computed all the ZIs on connection bases instead of degrees of the vertices and reported that the connection-based Zagreb indices (CBZIs) have larger ability to forecast the physical and chemical properties of molecular structures of chemistry than that of degree-based indices. After the initiation of CBZIs, all the researchers started working on measuring the properties of chemical structure with the help of these CBZIs. Cao et al. [23] computed ZCIs of molecular graphs. Sattar et al. [24–26] just discovered the CBZIs of dendrimer nanostars. Further, Ali et al. [27] estimated modified CBZIs for T-sum graphs in 2020. Haoer et al. [28] introduced the multiplicative leap ZIs. Javaid et al. [29] computed connection-based multiplicative ZIs (CBMZI) for various wheel networks. Du et al. [30] computed modified CBZIs for alkanes. Yang et al. [31] investigated the molecular characteristics of cubic carbon crystal formations. The motivation to this article is as follows.

(1) TIs, the numerical measure of a chemical compound, can describe the properties of chemical structure such as melting point, freezing point, density, pressure, tension, and temperature of chemical compounds. These TIs have much importance due to their wide range of applicability in reticular chemistry. They are efficient enough to characterize the topology of molecular compounds.

(2) Crystal cubic carbon structures are one of the important chemical structures due to the involvement of primary carbon element in it.

(3) Connection-based ZIs are more appropriate to anticipate the chemical and physical properties of chemical compounds than all the other introduced ZIs found in literature.

In this paper, we calculate the CBMZIs of crystal cubic carbon structure which is the most important allotrope of carbon. We find first CBMZI, second CBMZI, third CBMZI, and fourth CBMZI. We also compute the modified CBMZI, namely, modified first CBMZI, modified second CBMZI, and modified third CBMZI. This paper is organized as follows. Section 2 defines the basic definitions which are compulsory to understand and are helpful for the computation of main results. Section 3 consists of general expressions to compute the CBMZIs of structure of crystal cubic carbon. Section 4 draws the conclusions of this article.

2. Primary Definitions

This section involves the basic definitions which are helpful for the further calculations.

Definition 1 (see [11]). Let $G = (\mathscr{H}(G), \mathscr{T}(G))$ be a network, where $\mathscr{H}(G)$ denotes the set of vertices and $\mathscr{T}(G)$ denotes the set of edges, respectively. Then, the degree-based ZIs are defined as

(1) $\widehat{\mathfrak{Z}}_1(G) = \sum_{h\in\mathscr{H}(G)}(d_G(h))^2 = \sum_{ht\in\mathscr{T}(G)}(d_G(h) + d_G(t))$,

(2) $\widehat{\mathfrak{Z}}_2(G) = \sum_{ht\in\mathscr{T}(G)}(d_G(h) \times d_G(t))$,

where $d_G(h)$ and $d_G(t)$ show the degree of vertices h and t, respectively.

Definition 2 (see [22]). For a network G, connection-based Zagreb indices (CBZIs) are given as

(1) $\mathfrak{Z}_1\mathbb{C}\widetilde{I}(G) = \sum_{h\in\mathscr{H}(G)}(\tau_G(h))^2$,

(2) $\mathfrak{Z}_2\mathbb{C}\widetilde{I}(G) = \sum_{ht\in\mathscr{T}(G)}(\tau_G(h) \times \tau_G(t))$,

where $\tau_G(h)$ and $\tau_G(t)$ indicate the connection number (CN) of vertices h and t, respectively. These

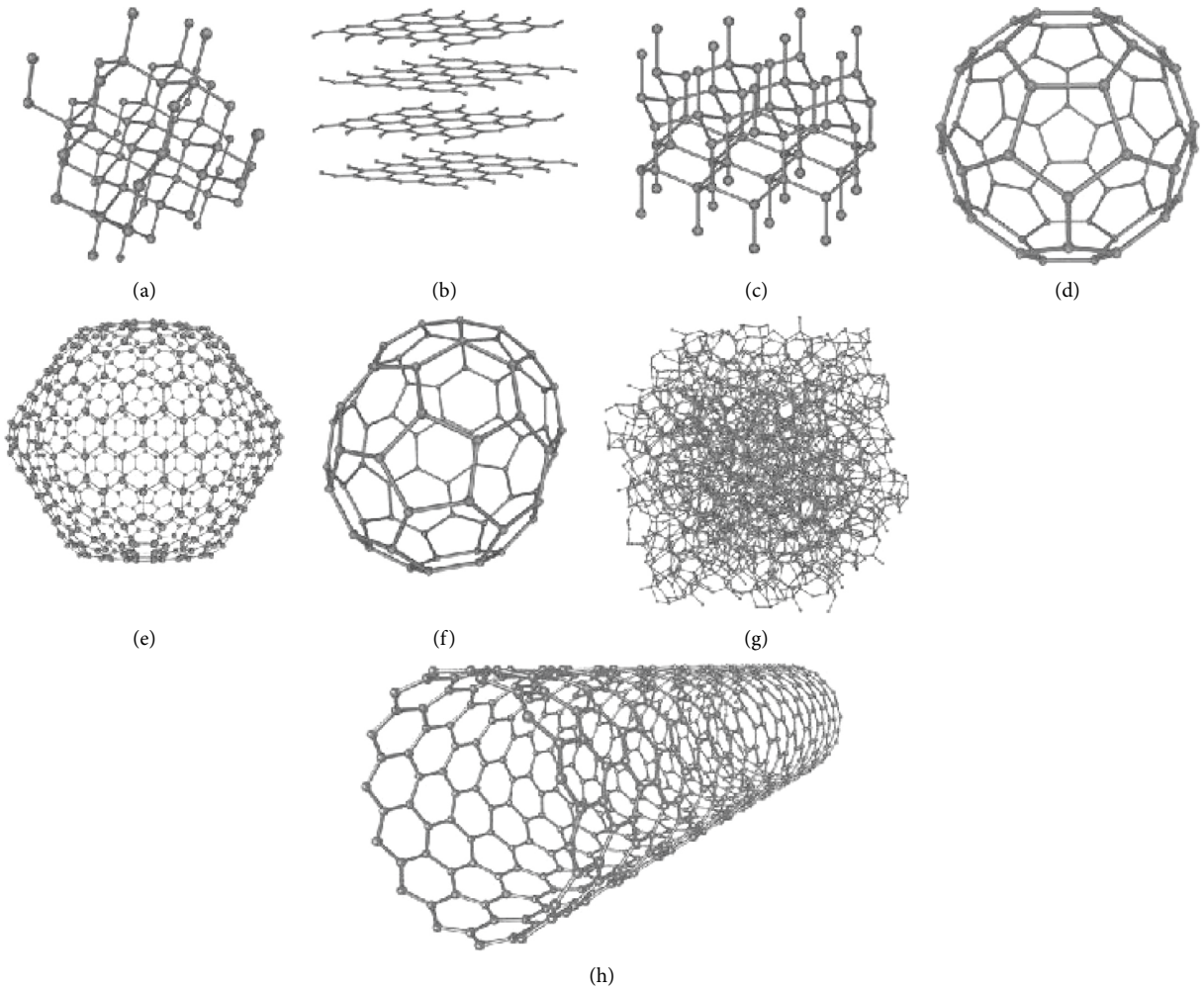

Figure 1: (a) Diamond. (b) Graphite. (c) Lonsdaleite. (d) C_{60}. (e) Fullerite. (f) C_{70}. (g) Amorphous carbon. (h) Carbon nanotube with single wall.

CBZIs are known as first CBZI and second CBZI, respectively.

Definition 3 (see [22, 27]). For a network G, the modified CBZIs can be given as

(1) $\mathfrak{Z}_1\mathbb{C}^*\widetilde{I}(G) = \sum_{ht\in\mathscr{T}(G)}(\tau_G(h) + \tau_G(t)) = \sum_{h\in\mathscr{H}(G)}(d_G(h)\ \tau_G(t))$,

(2) $\mathfrak{Z}_2\mathbb{C}^*\widetilde{I}(G) = \sum_{ht\in\mathscr{T}(G)}[d_G(h)\tau_G(t) + d_G(t)\tau_G(h)]$,

(3) $\mathfrak{Z}_3\mathbb{C}^*\widetilde{I}(G) = \sum_{ht\in\mathscr{T}(G)}[d_G(h)\tau_G(h) + d_G(t)\tau_G(t)]$.

These modified CBZIs are known as the modified first CBZI, modified second CBZI, and modified third CBZI, respectively.

Definition 4 (see [29]). For a network G, first CBMZI, second CBMZI, third CBMZI, and fourth CBMZI can be defined as

$$M\mathfrak{Z}_1\mathbb{C}\widetilde{I}(G) = \prod_{h\in\mathscr{H}(G)}(\tau_G(h))^2, \tag{1}$$

$$M\mathfrak{Z}_2\mathbb{C}\widetilde{I}(G) = \prod_{ht\in\mathscr{T}(G)}(\tau_G(h)\times\tau_G(t)), \tag{2}$$

$$M\mathfrak{Z}_3\mathbb{C}\widetilde{I}(G) = \prod_{h\in\mathscr{H}(G)}(d_G(h)\tau_G(h)), \tag{3}$$

$$M\mathfrak{Z}_4\mathbb{C}\widetilde{I}(G) = \prod_{ht\in\mathscr{T}(G)}(\tau_G(h) + \tau_G(t)). \tag{4}$$

Definition 5 (see [29]). For a network G, modified first CBMZI, modified second CBMZI, and modified third CBMZI can be defined as

$$M\mathfrak{Z}_1\mathscr{C}^*\tilde{I}(G) = \prod_{ht\in\mathscr{T}(G)} [d_G(h)\tau_G(t) + d_G(t)\tau_G(h)], \tag{5}$$

$$M\mathfrak{Z}_2\mathscr{C}^*\tilde{I}(G) = \prod_{ht\in\mathscr{T}(G)} [d_G(h)\tau_G(h) + d_G(t)\tau_G(t)], \tag{6}$$

$$M\mathfrak{Z}_3\mathscr{C}^*\tilde{I}(G) = \prod_{ht\in\mathscr{T}(G)} [d_G(h)\tau_G(h) \times d_G(t)\tau_G(t)]. \tag{7}$$

3. Connection-Based Multiplicative Zagreb Indices of Crystal Cubic Carbon Structure

The carbon's valency allows it to form a wide range of allotropes. Carbon is well recognized in the forms of graphite, bucky balls, diamond, etc. Graphite is the smooth, dark-colored substance found in lead of pencil. Diamonds, on the other hand, are extremely hard, typically clear, colorless, and extremely valuable jewels. Both of these structures are made up of carbon atom. In both of these structures, the carbon atom is piled differently and that is why both of these structures are very different to each other. Diamond is a tremendously strong substance made up of carbon atoms stacked densely together in a cubic crystal form. The strong bonds between the carbon atom make this structure very strong. There are many utilizations of these allotropes of carbon (for details, see [32]).

In this section, we deal with the computation of CBMZIs of this significant allotrope of carbon, namely, crystal cubic carbon structure ($CCC(j)$), where $j \geq 1$ is the level of the structure. Figure 2 depicts the molecular structure of rare stone cubic carbon structure $CCC(j)$ for the first level. For the next level, new 3D squares are linked at every terminal vertex of degree 3 of the previous first layer. Figure 3 depicts the second level of $CCC(j)$. Furthermore, the same technique is repeated to obtain the next level, and so on. Let $G = CCC(j)$ be a molecular network of $CCC(j)$ for $j \geq 2$. Molecular networks of $CCC(j)$ for $j = 2$ and $j = 3$ are shown in Figures 3 and 4, where we label the nodes (vertices) with their CNs. In Figures 5–7, we label the vertices with their degrees. The cardinality of vertices and edges in $CCC(j)$ is presented separately below.

$$\begin{aligned} |\mathscr{H}(CCC(j))| &= 8 + (8)^2 \sum_{k=2}^{j} \left(2^3 - 1\right)^{k-2}, \\ |\mathscr{T}(CCC(j))| &= 4\left[3 + 2\sum_{k=0}^{j-2} \left(2^3 - 1\right)^{k} + 24\left(2^3 - 1\right)^{j-2} + 24\sum_{k=3}^{j} \left(2^3 - 1\right)^{k-3}\right]. \end{aligned} \tag{8}$$

For our convenience, we divide the structure of G into three categories as given below.

(1) Basic cube: the cube which lies in the center of the molecular network of $CCC(j)$ is considered to be basic cube.

(2) Outer layer of cubes: the layer of cubes in which every cube has seven vertices with CN 6 is considered to be the outer layer of cubes.

(3) Central layer of cubes: the layer of cubes which is not the outer layer of cubes is said to be central layer of cube.

Theorem 1. *Consider a network $G = CCC(j)$ for $j \geq 2$. Then, the first CBMZI is equal to*

$$M\mathfrak{Z}_1\mathbb{C}\tilde{I}(G) = [36]^{8\left(2^3-1\right)^{j-1}} \times [81]^{8\left(2^3-1\right)^{j-2}} \times [144]^{\left(8+(8)^2\sum_{k=2}^{j}\left(2^3-1\right)^{k-2} - 8^2\left(2^3-1\right)^{j-2}\right)}. \tag{9}$$

Proof. In order to find the first CBMZI, we classify the collection of vertices based on their CNs into three classes. We have

$$\begin{aligned} \mathscr{H}_1 &= \{h \in \mathscr{H}\colon \tau_G(h) = 6\}, \\ \mathscr{H}_2 &= \{h \in \mathscr{H}\colon \tau_G(h) = 9\}, \\ \mathscr{H}_3 &= \{h \in \mathscr{H}\colon \tau_G(h) = 12\}. \end{aligned} \tag{10}$$

The cardinalities of $\mathscr{H}_1$, $\mathscr{H}_2$, and $\mathscr{H}_3$ are

$$\begin{aligned} |\mathscr{H}_1(G)| &= 8 \times \left(2^3 - 1\right)^{j-1}, \\ |\mathscr{H}_2(G)| &= 8 \times \left(2^3 - 1\right)^{j-2}, \\ |\mathscr{H}_3(G)| &= 8 + (8)^2 \sum_{k=2}^{j} \left(2^3 - 1\right)^{k-2} - 8^2\left(2^3 - 1\right)^{j-2}. \end{aligned} \tag{11}$$

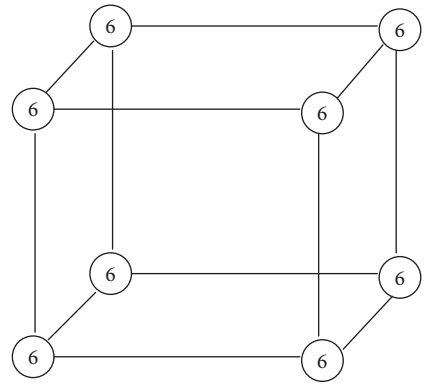

Figure 2: CCC(1) along with the labeling of CN 6 on the vertices of all the cubes.

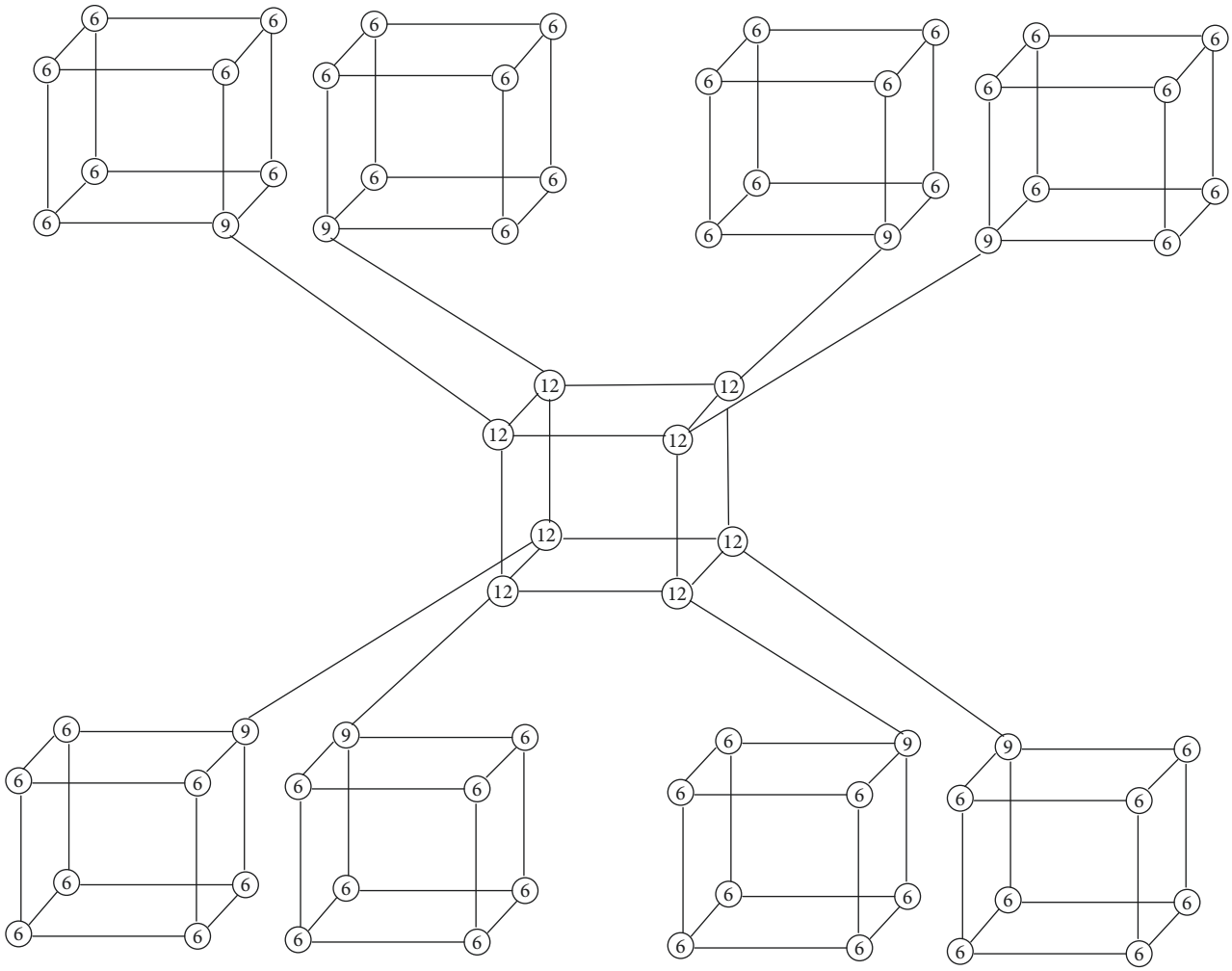

Figure 3: CCC(2) along with the labeling of CNs 6, 9, and 12 on the vertices of all the cubes.

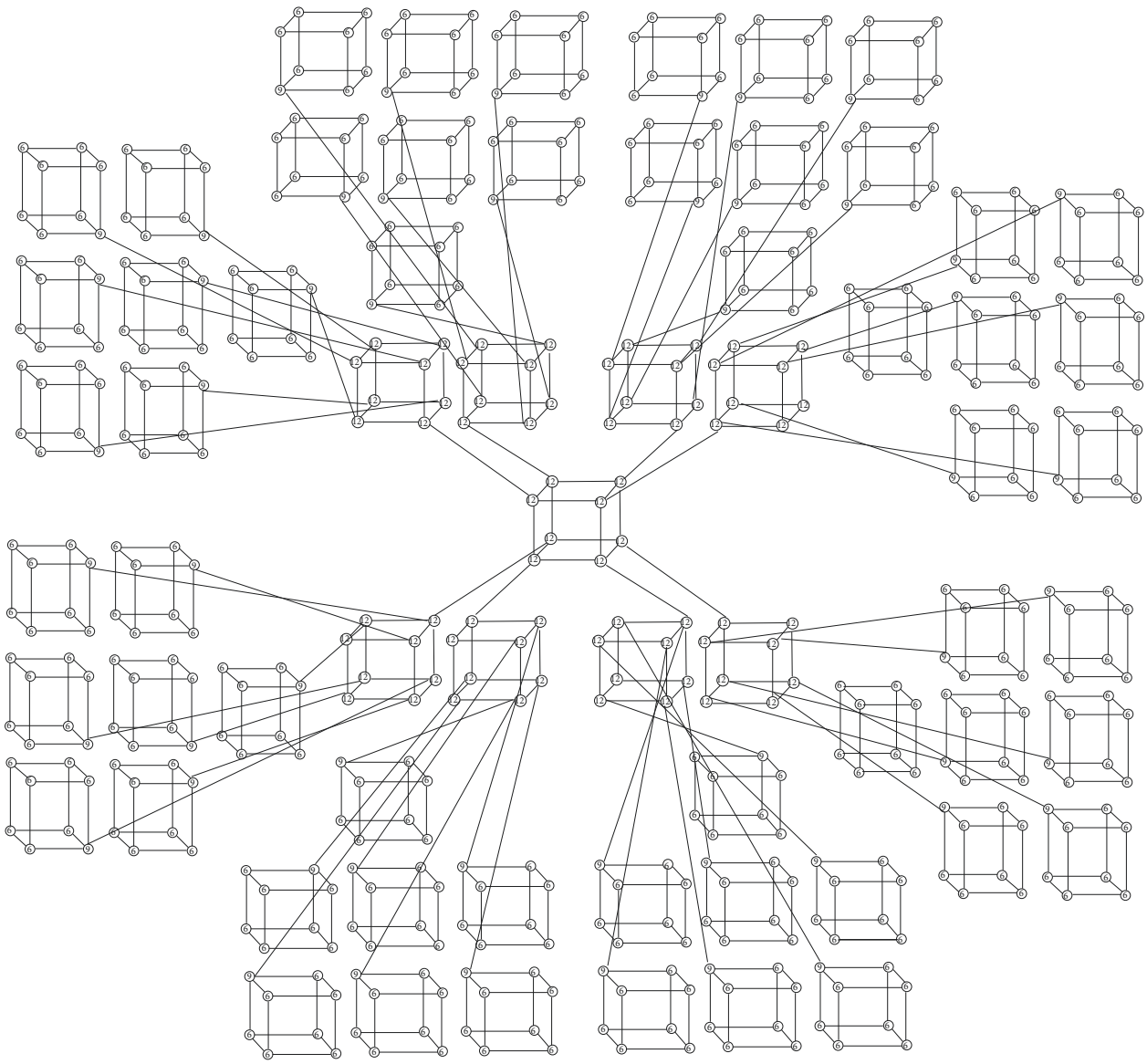

Figure 4: CCC(3) along with the labeling of CNs 6, 9, and 12 on the vertices of all the cubes.

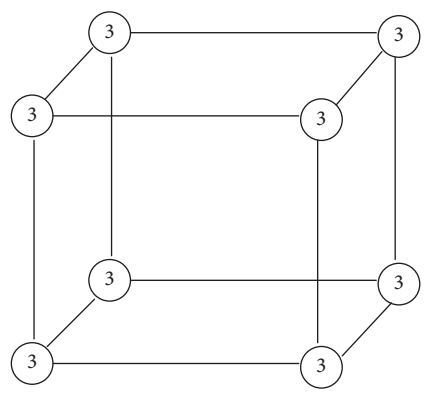

Figure 5: CCC(1) along with the labeling of degree 3 on the vertices of all the cubes.

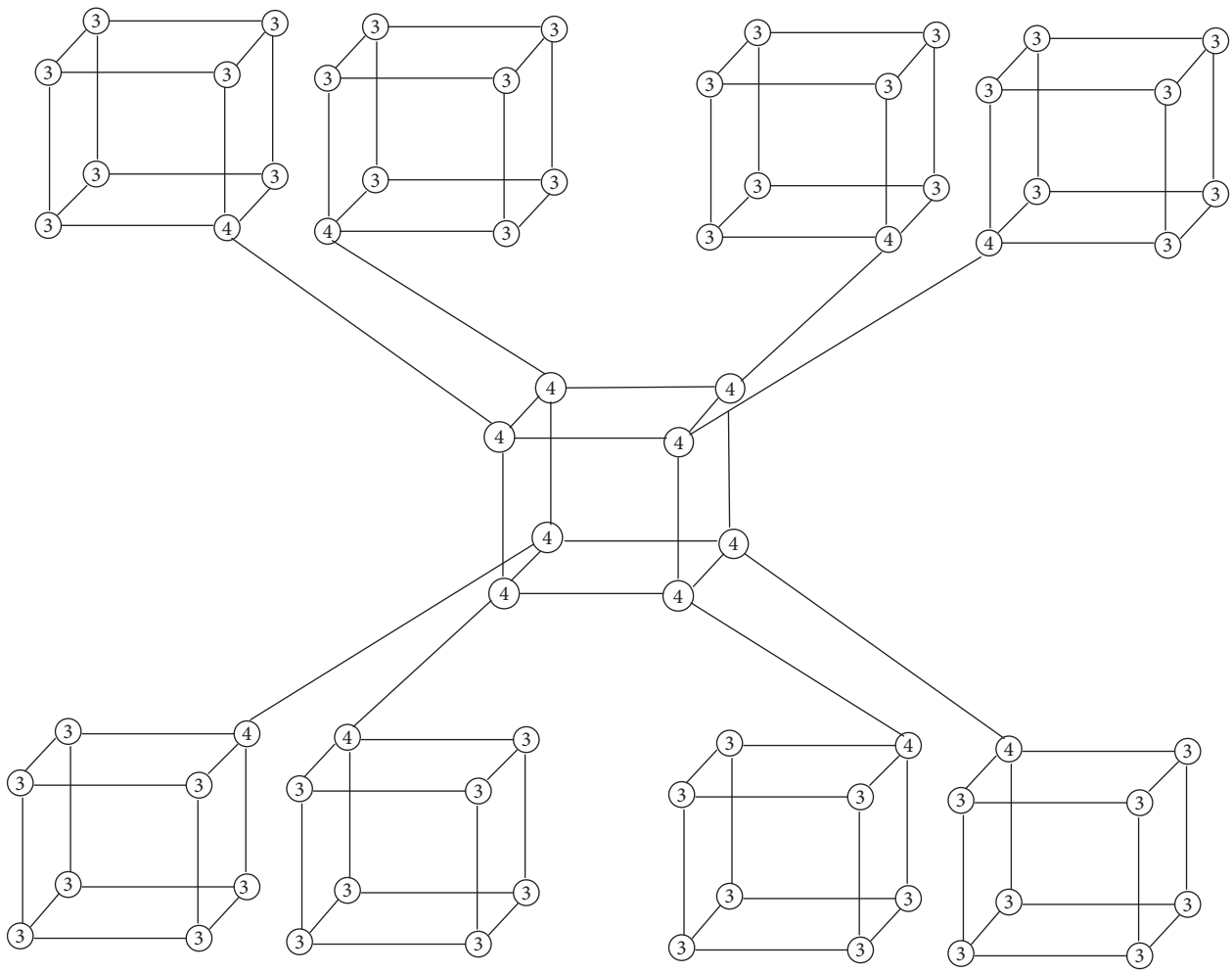

Figure 6: CCC(2) along with the labeling of degrees 3 and 4 on the vertices of all the cubes.

Now, by using equation (1), we get

$$
\begin{aligned}
M\mathfrak{Z}_1\mathbb{C}\tilde{I}(G) &= \prod_{h\in\mathscr{H}(G)} (\tau_G(h))^2, \\
&= \left[6^2\right]^{|\mathscr{H}_1(G)|} \times \left[9^2\right]^{|\mathscr{H}_2(G)|} \times \left[12^2\right]^{|\mathscr{H}_3(G)|}, \\
&= \left[6^2\right]^{\left(8\left(2^3-1\right)^{j-1}\right)} \times \left[9^2\right]^{\left(8\left(2^3-1\right)^{j-2}\right)} \\
&\quad \times \left[12^2\right]^{\left(8+(8)^2\sum_{k=2}^{j}\left(2^3-1\right)^{k-2}-8^2\left(2^3-1\right)^{j-2}\right)}, \\
&= [36]^{\left(8\left(2^3-1\right)^{j-1}\right)} \times [81]^{\left(8\left(2^3-1\right)^{j-2}\right)} \\
&\quad \times [144]^{\left(8+(8)^2\sum_{k=2}^{j}\left(2^3-1\right)^{k-2}-8^2\left(2^3-1\right)^{j-2}\right)}, \\
&= [36]^{8\left(2^3-1\right)^{j-1}} \times [81]^{8\left(2^3-1\right)^{j-2}} \times [144]^{\left(8+(8)^2\sum_{k=2}^{j}\left(2^3-1\right)^{k-2}-8^2\left(2^3-1\right)^{j-2}\right)}.
\end{aligned}
\tag{12}
$$

□

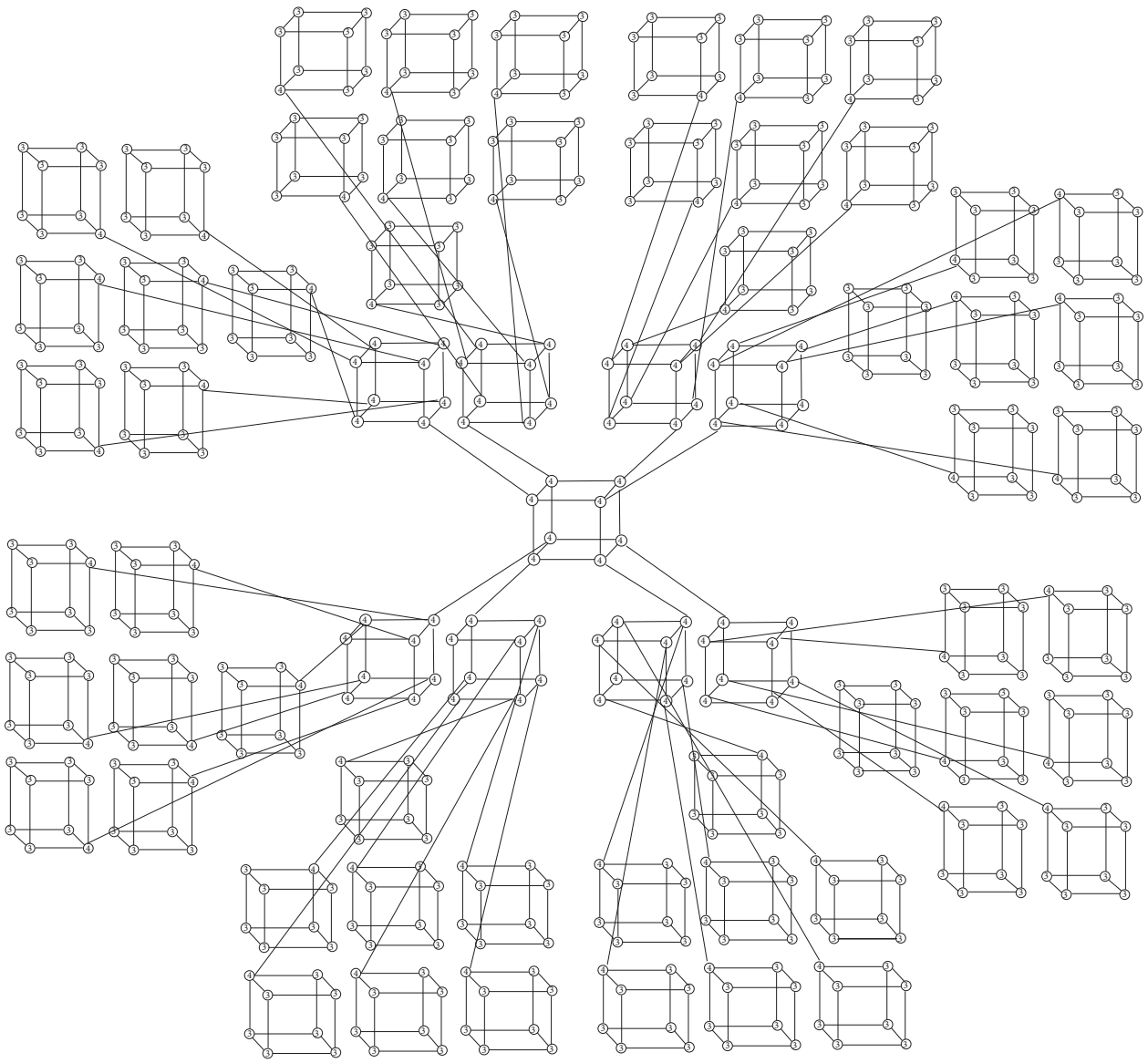

Figure 7: CCC(3) along with the labeling of degrees 3 and 4 on the vertices of all the cubes.

Theorem 2. *Consider a network $G = CCC(j)$ for $j \geq 2$. Then, the second CBMZI is equal to*

$$M\mathfrak{Z}_2\mathbb{C}\tilde{I}(G) = [36]^{72(2^3-1)^{j-2}} \times [54]^{24(2^3-1)^{j-2}} \times [108]^{\left(8\sum_{k=0}^{j-2}(2^3-1)^k\right)} \times [144]^{\left(12+96\sum_{k=3}^{j}(2^3-1)^{k-3}\right)}. \tag{13}$$

Proof. Firstly, we divide the edges into four classes with respect to their CNs. We have

$$\begin{aligned}
\mathscr{C}_1 &= \mathscr{T}_{(6,6)}(G) = \{ht \in \mathscr{T}\colon \tau_G(h) = 6, \tau_G(t) = 6\},\\
\mathscr{C}_2 &= \mathscr{T}_{(6,9)}(G) = \{ht \in \mathscr{T}\colon \tau_G(h) = 6, \tau_G(t) = 9\},\\
\mathscr{C}_3 &= \mathscr{T}_{(9,12)}(G) = \{ht \in \mathscr{T}\colon \tau_G(h) = 9, \tau_G(t) = 12\},\\
\mathscr{C}_4 &= \mathscr{T}_{(12,12)}(G) = \{ht \in \mathscr{T}\colon \tau_G(h) = 12, \tau_G(t) = 12\}.
\end{aligned} \tag{14}$$

To find second CBMZI, we find the cardinalities of above partitioned edges. For this, we first find the number of edges in basic cube, outer layer of the vertices, and central layer of the cubes. After some simple calculation, we have

$$\begin{aligned}&\text{total edges in basic cube} = 12,\\ &\text{total edges in outer layer} = 96\left(2^3-1\right)^{j-2},\\ &\text{total edges in central layer} = 96\sum_{k=3}^{j}\left(2^3-1\right)^{k-3}.\end{aligned} \tag{15}$$

The edges which are not the part of any cube are considered to be free edges. The total number of free edges is $8\sum_{k=0}^{j-2}(2^3-1)^k$. Now, we compute $|\mathscr{T}_{(6,6)}(G)|$. As from the network of G, we can observe that $(6,6)$–type edges only exist in the outer layer of the cubes. After some easy calculation, we get

$$|\mathscr{T}_{(6,6)}(G)| = 72\times\left(2^3-1\right)^{j-2}. \tag{16}$$

Now, we compute $|\mathscr{T}_{(6,9)}(G)|$. Similar to $(6,6)$–type edges, $(6,9)$–type edges also lie only in outer layer of the cubes. Thus, we have

$$\begin{aligned}|\mathscr{T}_{(6,9)}(G)| &= 96\left(2^3-1\right)^{j-2}-72\left(2^3-1\right)^{j-2},\\ &= 24\left(2^3-1\right)^{j-2}.\end{aligned} \tag{17}$$

Next, we find the number of edges with CNs $(9,12)$. We can see that only the free edges have CNs (9,12). The total number of free edges is $8\sum_{k=0}^{j-2}(2^3-1)^k$. Thus, we have

$$|\mathscr{T}_{(9,12)}(G)| = 8\sum_{k=0}^{j-2}\left(2^3-1\right)^k. \tag{18}$$

Lastly, we compute $|\mathscr{T}_{(12,12)}(G)|$. It can be easily observed from the network of G that basic cube and central layer of cubes contain all those edges which have CNs (12,12). Thus, the total number of $(12,12)$ edges must be the sum of edges of basic cube and the edges of central layer of the cubes. Hence, we have

$$|\mathscr{T}_{(12,12)}(G)| = 12+96\sum_{k=3}^{j}\left(2^3-1\right)^{k-3}. \tag{19}$$

Adding all types of edges gives the cardinality of edges of G. Now, by using equation (2), we have

$$\begin{aligned}M\mathfrak{Z}_2\mathbb{C}\tilde{I}(G) &= \prod_{ht\in\mathscr{T}(G)}\left(\tau_G(h)\times\tau_G(t)\right)\\ &= [6\times6]^{|\mathscr{T}_{(6,6)}(G)|}\times[6\times9]^{|\mathscr{T}_{(6,9)}(G)|}\times[9\times12]^{|\mathscr{T}_{(9,12)}(G)|}\times[12\times12]^{|\mathscr{T}_{(12,12)}(G)|}\\ &= [6\times6]^{\left(72\left(2^3-1\right)^{j-2}\right)}\times[6\times9]^{\left(24\left(2^3-1\right)\right)^{j-2}}\times[9\times12]^{\left(8\sum_{k=0}^{j-2}\left(2^3-1\right)^k\right)}\times[12\times12]^{\left(12+96\sum_{k=3}^{j}\left(2^3-1\right)^{k-3}\right)}\\ &= [36]^{72\left(2^3-1\right)^{j-2}}\times[54]^{24\left(2^3-1\right)^{j-2}}\times[108]^{\left(8\sum_{k=0}^{j-2}\left(2^3-1\right)^k\right)}\times[144]^{\left(12+96\sum_{k=3}^{j}\left(2^3-1\right)^{k-3}\right)}.\end{aligned} \tag{20}$$

□

Theorem 3. *Consider a network $G = CCC(j)$ for $j \geq 2$. Then, the third CBMZI is equal to*

$$M\mathfrak{Z}_3\mathbb{C}\tilde{I}(G) = [18]^{8\times\left(2^3-1\right)^{j-1}}\times[36]^{8\times\left(2^3-1\right)^{j-2}}\times[48]^{8+(8)^2\sum_{k=2}^{j}\left(2^3-1\right)^{k-2}-8^2\left(2^3-1\right)^{j-2}}. \tag{21}$$

Proof. Before computing third CBMZI, we make the classes of vertices on the bases of their degrees. We have only two classes of vertices on the basis of degrees of vertices.

$$\begin{aligned}\mathscr{H}_1^d(G) &= \{h\in\mathscr{H}\colon d_G(h)=3\},\\ \mathscr{H}_2^d(G) &= \{h\in\mathscr{H}\colon d_G(h)=4\}.\end{aligned} \tag{22}$$

Now, we make the partitions of vertices with respect to the degrees and CNs of the vertices. We have

$$\begin{aligned}\mathscr{H}_1'(G) &= \{h\in\mathscr{H}\colon d_G(h)=3,\tau_G(h)=3\},\\ \mathscr{H}_2'(G) &= \{h\in\mathscr{H}\colon d_G(h)=4,\tau_G(h)=9\},\\ \mathscr{H}_3'(G) &= \{h\in\mathscr{H}\colon d_G(h)=4,\tau_G(h)=12\}.\end{aligned} \tag{23}$$

The cardinalities of these vertices are given in the following:

$$\begin{aligned}
\left|\mathscr{H}_1'(G)\right| &= 8\times\left(2^3-1\right)^{j-1},\\
\left|\mathscr{H}_2'(G)\right| &= 8\times\left(2^3-1\right)^{j-2},\\
\left|\mathscr{H}_3'(G)\right| &= 8+(8)^2\sum_{k=2}^{j}\left(2^3-1\right)^{k-2}-8^2\left(2^3-1\right)^{j-2}.
\end{aligned} \tag{24}$$

By using equation (3), we get

$$\begin{aligned}
M\mathfrak{Z}_3\mathbb{C}\tilde{I}(G) &= \prod_{h\in\mathscr{H}(G)}\left(d_G(h)\tau_G(h)\right)\\
&= [3\times 6]^{\left|\mathscr{H}_1'(G)\right|}\times[4\times 9]^{\left|\mathscr{H}_2'(G)\right|}\times[4\times 12]^{\left|\mathscr{H}_3'(G)\right|}\\
&= [3\times 6]^{8\times\left(2^3-1\right)^{j-1}|}\times[4\times 9]^{8\times\left(2^3-1\right)^{j-2}|}\times[4\times 12]^{\left(8+(8)^2\sum_{k=2}^{j}\left(2^3-1\right)^{k-2}-8^2\left(2^3-1\right)^{j-2}\right)}\\
&= [18]^{8\times\left(2^3-1\right)^{j-1}}\times[36]^{8\times\left(2^3-1\right)^{j-2}}\times[48]^{\left(8+(8)^2\sum_{k=2}^{j}\left(2^3-1\right)^{k-2}-8^2\left(2^3-1\right)^{j-2}\right)}.
\end{aligned} \tag{25}$$

□

Theorem 4. *Consider a network $G = CCC(j)$ for $j \geq 2$. Then, the fourth CBMZI is equal to*

$$M\mathfrak{Z}_4\mathbb{C}\tilde{I}(G) = [12]^{72\left(2^3-1\right)^{j-2}}\times[15]^{24\left(2^3-1\right)^{j-2}}\times[21]^{\left(8\sum_{k=0}^{j-2}\left(2^3-1\right)^{k}\right)}\times[36]^{\left(12+96\sum_{k=3}^{j}\left(2^3-1\right)^{k-3}\right)}. \tag{26}$$

Proof. By placing the values of $\mathscr{T}_{(\tau_G(h),\tau_G(t))}$ in equation (4), we have

$$\begin{aligned}
M\mathfrak{Z}_4\mathbb{C}\tilde{I}(G) &= \prod_{ht\in\mathscr{T}(G)}\left(\tau_G(h)+\tau_G(t)\right), = [6+6]^{\left|\mathscr{T}_{(6,6)}(G)\right|}+[6+9]^{\left|\mathscr{T}_{(6,9)}(G)\right|}\times[9+12]^{\left|\mathscr{T}_{(9,12)}(G)\right|}\times[12+12]^{\left|\mathscr{T}_{(12,12)}(G)\right|}\\
&= [6+6]^{\left(72\left(2^3-1\right)^{j-2}\right)}\times[6+9]^{\left(24\left(2^3-1\right)\right)^{j-2}}\times[9+12]^{\left(8+\sum_{k=0}^{j-2}\left(2^3-1\right)^{k}\right)}\times[12+12]^{\left(12+96\sum_{k=3}^{j}\left(2^3-1\right)^{k-3}\right)}\\
&= [12]^{72\left(2^3-1\right)^{j-2}}\times[15]^{24\left(2^3-1\right)^{j-2}}\times[21]^{\left(8\sum_{k=0}^{j-2}\left(2^3-1\right)^{k}\right)}\times[36]^{\left(12+96\sum_{k=3}^{j}\left(2^3-1\right)^{k-3}\right)}.
\end{aligned} \tag{27}$$

□

Theorem 5. *Consider a network $G = CCC(j)$ for $j \geq 2$. Then, the modified first CBMZI is equal to*

$$M\mathfrak{Z}_1\mathbb{C}^*\tilde{I}(G) = [36]^{72\left(2^3-1\right)^{j-2}}\times[51]^{24\left(2^3-1\right)^{j-2}}\times[84]^{\left(8\sum_{k=0}^{j-2}\left(2^3-1\right)^{k}\right)}\times[96]^{\left(12+96\sum_{k=3}^{j}\left(2^3-1\right)^{k-3}\right)}. \tag{28}$$

Proof. Firstly, we divide the edges into three classes with respect to their degrees. We have

$$\begin{aligned}\mathscr{C}_1 &= \mathscr{T}^d_{(3,3)}(G) = \{ht \in \mathscr{M}:\ d_G(h) = 3,\ d_G(t) = 3\},\\ \mathscr{C}_2 &= \mathscr{T}^d_{(3,4)}(G) = \{ht \in \mathscr{M}:\ d_G(h) = 3,\ d_G(t) = 4\},\\ \mathscr{C}_3 &= \mathscr{T}^d_{(4,4)}(G) = \{ht \in \mathscr{M}:\ d_G(h) = 4,\ d_G(t) = 4\}.\end{aligned} \tag{29}$$

In order to calculate the modified first CBMZI, first we need to calculate the number of edges on the basis of their degrees of incident vertices. Initially, we calculate $|\mathscr{T}^d_{(3,3)}(G)|$. It can be observed that (3,3)-type edges only lie in the cubes of the outer layer. For simple calculations, we have

$$\left|\mathscr{T}^d_{(3,3)}(G)\right| = 72\left(2^3 - 1\right)^{j-2}. \tag{30}$$

Now, we compute $|\mathscr{T}^d_{(3,4)}(G)|$. Similar to (3,3)-type edges of G, (3,4)-type edges also exist only in the cubes of the outer layer of G. The number of $(3,4)-$type edges must be equal to the total number of edges in the cubes of outer layer minus the (3,3)-type edges present in the cubes of outer layer of G. Thus, we have

$$\begin{aligned}\left|\mathscr{T}^d_{(3,4)}(\text{ outer layer of the cubes})\right| &= 96\left(2^3 - 1\right)^{j-2},\\ \left|\mathscr{T}^d_{(3,3)}(\text{ outer layer of the cubes})\right| &= 72\left(2^3 - 1\right)^{j-2},\\ \left|\mathscr{T}^d_{(3,4)}(G)\right| &= 96\left(2^3 - 1\right)^{j-2} - 72\left(2^3 - 1\right)^{j-2},\\ &= 24\left(2^3 - 1\right)^{j-2}.\end{aligned} \tag{31}$$

Lastly, we compute $|\mathscr{T}^d_{(4,4)}(G)|$. One can see from the network of G that the basic cube and central layer of cubes have all those edges which have CNs (4,4). Also, all the free edges are (4,4)-type edges. Thus, the total number of $(4,4)-$type edges must be the sum of edges of basic cube and the edges of central layer of the cubes plus all the free edges. Hence, we have

$$\begin{aligned}\text{Total edges in basic cube} &= 12,\\ \text{Number of edges in central layer} &= 96\sum_{k=3}^{j}\left(2^3 - 1\right)^{k-3},\\ \text{Total free edges} &= 8\sum_{k=0}^{j-2}\left(2^3 - 1\right)^{k},\\ \left|\mathscr{T}^d_{(4,4)}(G)\right| &= 12 + 96\sum_{k=3}^{j}\left(2^3 - 1\right)^{k-3} + 8\sum_{k=0}^{j-2}\left(2^3 - 1\right)^{k}.\end{aligned} \tag{32}$$

To compute the modified first CBMZI, we split the classified number of edges on degree bases with respect to the number of edges on connection bases. The partitioning of degree-based edges with respect to connection-based edges is shown in Table 1.

To compute the modified first CBZI, we are not concerning with degrees or CNs of edges separately, instead we are dealing with both degrees and CNs of the edges . From Figures 4 and 7, we can see that there are total four such partitions of edges as given below.

$$\begin{aligned}\mathscr{T}_{(3,3)(6,6)}(G) &= \{ht \in \mathscr{T}:\ d_G(h) = 3, \tau_G(h) = 6, d_G(t) = 3, \tau_G(t) = 6\},\\ \mathscr{T}_{(3,4)(6,9)}(G) &= \{ht \in \mathscr{T}:\ d_G(h) = 3, \tau_G(h) = 6, d_G(h) = 4, \tau_G(t) = 9\},\\ \mathscr{T}_{(4,4)(9,12)}(G) &= \{ht \in \mathscr{T}:\ d_G(h) = 4, \tau_G(h) = 9, d_G(h) = 4, \tau_G(t) = 12\},\\ \mathscr{T}_{(4,4)(12,12)}(G) &= \{ht \in \mathscr{T}:\ d_G(h) = 4, \tau_G(h) = 12, d_G(h) = 4, \tau_G(t) = 12\}.\end{aligned} \tag{33}$$

Table 1: Partitioning of degree-based edges with respect to connection-based edges.

$\lvert\mathcal{T}^{d}_{(d_G(h),d_G(t))}(G)\rvert$ (degree based)	$\lvert\mathcal{T}_{(\tau_G(h),\tau_G(t))}(G)\rvert$ (connection based)
$\lvert\mathcal{T}^{d}_{(3,3)}(G)\rvert = 72(2^3-1)^{j-2}$	$\lvert\mathcal{T}_{(6,6)}(G)\rvert = 72(2^3-1)^{j-2}$
$\lvert\mathcal{T}^{d}_{(3,4)}(G)\rvert = 24(2^3-1)^{j-2}$	$\lvert\mathcal{T}_{(6,9)}(G)\rvert = 24(2^3-1)^{j-2}$
$\lvert\mathcal{T}^{d}_{(4,4)}(G)\rvert = 8\sum_{k=0}^{j-2}(2^3-1)^{k}$	$\lvert\mathcal{T}_{(9,12)}(G)\rvert = 8\sum_{k=0}^{j-2}(2^3-1)^{k}$
$\lvert\mathcal{T}^{d}_{(4,4)}(G)\rvert = 12 + 96\sum_{k=3}^{j}(2^3-1)^{k-3}$	$\lvert\mathcal{T}_{(12,12)}(G)\rvert = 12 + 96\sum_{k=3}^{j}(2^3-1)^{k-3}$

Table 2: Cardinalities of partitioned edges on degree and connection bases.

$\mathcal{T}_{(d(h),d(t))(\tau(h),\tau(t))}(G)$	$\lvert\mathcal{T}_{(d(h),d(t))(\tau(h),\tau(t))}(G)\rvert$
$\lvert\mathcal{T}_{(3,3)(6,6)}(G)\rvert$	$72(2^3-1)^{j-2}$
$\lvert\mathcal{T}_{(3,4)(6,9)}(G)\rvert$	$24(2^3-1)^{j-2}$
$\lvert\mathcal{T}_{(4,4)(9,12)}(G)\rvert$	$8\sum_{k=0}^{j-2}(2^3-1)^{k}$
$\lvert\mathcal{T}_{(4,4)(12,12)}(G)\rvert$	$12 + 96\sum_{k=3}^{j}(2^3-1)^{k-3}$

By using Table 1, the cardinalities of these partitioned vertices are displayed in Table 2.

By using equation (5), we get

$$\begin{aligned}
M\mathfrak{Z}_1\mathbb{C}^{*}\tilde{I}(G) &= \prod_{ht\in\mathcal{T}(G)}\left[d_G(h)\tau_G(t)+d_G(t)\tau_G(h)\right]\left[(4)(12)+(4)(9)\right]^{\lvert\mathcal{T}_{(4,4)(9,12)}(G)\rvert}\times\left[(4)(12)+(4)(12)\right]^{\lvert\mathcal{T}_{(4,4)(12,12)}(G)\rvert}\\
&= \left[(3)(6)+(3)(6)\right]^{72(2^3-1)^{j-2}}\times\left[(3)(9)+(4)(6)\right]^{24(2^3-1)^{j-2}}+\left[(4)(12)+(4)(9)\right]^{\left(8\sum_{k=0}^{j-2}(2^3-1)^{k}\right)}\\
&\quad\times\left[(4)(12)+(4)(12)\right]^{\left(12+96\sum_{k=3}^{j}(2^3-1)^{k-3}\right)}\\
&= \left[(3)(6)+(3)(6)\right]^{\lvert\mathcal{T}_{(3,3)(6,6)}(G)\rvert}\times\left[(3)(9)+(4)(6)\right]^{\lvert\mathcal{T}_{(3,4)(6,9)}(G)\rvert}+\\
&= \left[18+18\right]^{72(2^3-1)^{j-2}}\times\left[27+24\right]^{24(2^3-1)^{j-2}}+\left[48+36\right]^{\left(8\sum_{k=0}^{j-2}(2^3-1)^{k}\right)}\times\left[48+48\right]^{\left(12+96\sum_{k=3}^{j}(2^3-1)^{k-3}\right)}\\
&= \left[36\right]^{72(2^3-1)^{j-2}}\times\left[51\right]^{24(2^3-1)^{j-2}}\times\left[84\right]^{\left(8\sum_{k=0}^{j-2}(2^3-1)^{k}\right)}\times\left[96\right]^{\left(12+96\sum_{k=3}^{j}(2^3-1)^{k-3}\right)}.
\end{aligned}\tag{34}$$

□

Theorem 6. *Consider a network $G = CCC(j)$ for $j \geq 2$. Then, the modified second CBMZI is*

$$M\mathfrak{Z}_2\mathbb{C}^{*}\tilde{I}(G) = \left[36\right]^{\left(72(2^3-1)^{j-2}\right)}\times\left[54\right]^{\left(24(2^3-1)^{j-2}\right)}\times\left[84\right]^{\left(8\sum_{k=0}^{j-2}(2^3-1)^{k}\right)}\times\left[96\right]^{\left(12+96\sum_{k=3}^{j}(2^3-1)^{k-3}\right)}.\tag{35}$$

Proof. By using equation (6), we get

$$\begin{aligned}
M\mathfrak{Z}_2\mathbb{C}^{*}\tilde{I}(G) &= \prod_{ht\in\mathcal{T}(G)}\left[d_G(h)\tau_G(h)+d_G(t)\tau_G(t)\right]\\
&= \left[(3)(6)+(3)(6)\right]^{\lvert\mathcal{T}_{(3,3)(6,6)}(G)\rvert}\times\left[(3)(6)+(4)(9)\right]^{\lvert\mathcal{T}_{(3,4)(6,9)}(G)\rvert}\times\left[(4)(9)+(4)(12)\right]^{\lvert\mathcal{T}_{(4,4)(9,12)}(G)\rvert}\times\left[(4)(12)+(4)(12)\right]^{\lvert\mathcal{T}_{(4,4)(12,12)}(G)\rvert}\\
&= \left[(3)(6)+(3)(6)\right]^{\left(72(2^3-1)^{j-2}\right)}\times\left[(3)(6)+(4)(9)\right]^{\left(24(2^3-1)^{j-2}\right)}\times\left[(4)(9)+(4)(12)\right]^{\left(8\sum_{k=0}^{j-2}(2^3-1)^{k}\right)}\\
&\quad\times\left[(4)(12)+(4)(12)\right]^{\left(12+96\sum_{k=3}^{j}(2^3-1)^{k-3}\right)}\\
&= \left[18+18\right]^{\left(72(2^3-1)^{j-2}\right)}\times\left[18+36\right]^{\left(24(2^3-1)^{j-2}\right)}\times\left[36+48\right]^{\left(8\sum_{k=0}^{j-2}(2^3-1)^{k}\right)}\times\left[48+48\right]^{\left(12+96\sum_{k=3}^{j}(2^3-1)^{k-3}\right)}\\
&= \left[36\right]^{\left(72(2^3-1)^{j-2}\right)}\times\left[54\right]^{\left(24(2^3-1)^{j-2}\right)}\times\left[84\right]^{\left(8\sum_{k=0}^{j-2}(2^3-1)^{k}\right)}\times\left[96\right]^{\left(12+96\sum_{k=3}^{j}(2^3-1)^{k-3}\right)}.
\end{aligned}\tag{36}$$

□

Theorem 7. *Consider a network $G = CCC(j)$ for $j \geq 2$. Then, the modified third CBMZI is equal to*

$$M\mathfrak{Z}_3\mathbb{C}^*\tilde{I}(G) = [324]^{\left(72(2^3-1)^{j-2}\right)} \times [648]^{\left(24(2^3-1)^{j-2}\right)} \times [1728]^{\left(8\sum_{k=0}^{j-2}(2^3-1)^k\right)} \times [2304]^{\left(12+96\sum_{k=3}^{j}(2^3-1)^{k-3}\right)}. \tag{37}$$

Proof. By using equation (7), we get

$$\begin{aligned}
M\mathfrak{Z}_3\mathbb{C}^*\tilde{I}(G) &= \prod_{ht\in\mathcal{T}(G)} [d_G(h)\tau_G(h) \times d_G(t)\tau_G(t)] \\
&= [(3)(6)\times(3)(6)]^{|\mathcal{T}_{(3,3)(6,6)}(G)|} \times [(3)(6)\times(4)(9)]^{|\mathcal{T}_{(3,4)(6,9)}(G)|} \times [(4)(9)\times(4)(12)]^{|\mathcal{T}_{(4,4)(9,12)}(G)|} \\
&\quad \times [(4)(12)\times(4)(12)]^{|\mathcal{T}_{(4,4)(12,12)}(G)|} \\
&= [(3)(6)\times(3)(6)]^{\left(72(2^3-1)^{j-2}\right)} \times [(3)(6)\times(4)(9)]^{\left(24(2^3-1)^{j-2}\right)} \times [(4)(9)\times(4)(12)]^{\left(8\sum_{k=0}^{j-2}(2^3-1)^k\right)} \\
&\quad \times [(4)(12)\times(4)(12)]^{\left(12+96\sum_{k=3}^{j}(2^3-1)^{k-3}\right)} \\
&= [18\times18]^{\left(72(2^3-1)^{j-2}\right)} \times [18\times36]^{\left(24(2^3-1)^{j-2}\right)} \times [36\times48]^{\left(8\sum_{k=0}^{j-2}(2^3-1)^k\right)} \times [48\times48]^{\left(12+96\sum_{k=3}^{j}(2^3-1)^{k-3}\right)} \\
&= [324]^{\left(72(2^3-1)^{j-2}\right)} \times [648]^{\left(24(2^3-1)^{j-2}\right)} \times [1728]^{\left(8\sum_{k=0}^{j-2}(2^3-1)^k\right)} \times [2304]^{\left(12+96\sum_{k=3}^{j}(2^3-1)^{k-3}\right)}.
\end{aligned} \tag{38}$$

□

4. Conclusion

In this study, we have found the general expressions to compute the TIs of the allotrope of carbon, namely, crystal structure of carbon. TIs help the researchers for the examination and manipulation of chemical structural information. Here, we have calculated various TIs, named as first CBMZI and second CBMZI. We have also computed modified first CBMZI, modified second CBMZI, and modified third CBMZI. This computational study will make it easier for the researchers to understand the selected structure and will encourage others to concentrate on the organic networks. The mathematical method considered here is efficient to examine the physical and chemical properties of the considered network.

Future Directions. In future, we are interested in computing the connection-based Zagreb indices for other types of chemical structures.

Data Availability

The data used to support the findings of this study are included within this article. However, the reader may contact the corresponding author for more details on the data.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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