Research Article

Study of Generalized Hourglass Section in Carbon Nanocone via Connection Number

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1. Introduction

In the theoretical branch of chemistry, molecular quantities are important for modeling structural information of different molecules. The purpose for getting this information is to capture physical and chemical properties of the molecules. To attain this, a chemical structure of a molecule is presented as graphs, and the molecular quantities obtained from a particular chemical structure are graph invariants under graph isomorphism. In the mathematical branch of chemistry, this study is termed as quantitative structural activity relationship (QSAR). Predicting electron energy and melting (boiling) point for a structure are primary applications of these studies [1].

In discrete branch of mathematics, studying mathematical structures by modeling pairwise relations between sets of objects results in graphs. Simply, a graph consists of some vertices, which are joined by edges. Commonly, the set of vertices in a graph $G$ is described by $V$, whereas the set of edges is represented by $E$. Chemical graph theory is a branch of mathematics which combines graph theory and chemistry. Graph theory is used to mathematically model molecules in order to gain insight into the physical properties of these chemical compounds. In this branch, a chemical structure for a compound is visualized as a unique form of a graph by showing its atoms as vertices and bonds between atoms as edges. This is a simple transformation of a structure into a graph which helps chemists to study physical and chemical structural properties for a particular network [2]. Very recently, a new two-dimensional bilayered naturally existing network of germanium phosphide is topologically explained in [3]. Some degree-based topological indices for p-type benzene ring for a two-dimensional network are given in [4]. A computer paradigm cellular neural network is explained by a new kind of dominating topological invariants by Ejaz et al. [5].

In 1972, Ivan Gutman and Nenad Trinajstic [6] very firstly defined a numeric quantity while studying the electron energy of a molecule. Later on, this quantity will have been called as the Zagreb index. It depends on the number of...
bonds (edges) connected to an atom. Particularly, the number of bonds attached to an atom is called degree, and Zagreb index is purely based on degrees of all atoms in a structure. After this, these same mathematicians defined another quantity while studying molecular branching of orbitals which is called the second Zagreb index. With the passage of time, the abovementioned quantities would be termed as the first and second Zagreb indices by many graph theorists and chemists. More than hundreds of researchers did work on it and published their work in highly reputed journals [7].

In [1, 8], these two quantities are modified and redefined as nodal quantities on the basis of connection numbers, and this experiment shows very effective results in different aspects. As we know that the number of edges (bonds) is the degree of an atom (vertex), similarly, the second degree is the number of edges from a particular vertex to a vertex at a distance two. In other words, for a vertex $u$ in a graph, the number of vertices at a distance two is called the connection number for $u$ and represented as $\tau_2(u)$. In the following, we will define these modified versions of Zagreb indices and are termed as the first Zagreb connection number ($ZC_1$), second Zagreb connection number ($ZC_2$), and more modified type of first Zagreb as first modified connection number ($ZC_1^*$).

\[ ZC_1 = \sum_{u \in V} \tau_2(u), \]  
\[ ZC_2 = \sum_{u \in V} (\tau_2(u)), \]  
\[ ZC_1^* = \sum_{u \in V} (\tau_2(u) + \tau_3(u)). \]  

2. Carbon Nanocone

Round about in 1968, the first appearance of a carbon nanocone comes under observation by naturally existing graphite surface. The attraction of these structures is its applications in biosensors, energy and gas storage, nano-electric devices, and many more. These nanocones are carbon-consisting networks which are infinite undirected planar structures in theory of graphs [9].

Carbon nanomaterials have drawn focusable attention and attraction during the last two decades because of its effective physical applications in nanotechnology as emerging materials of splendid practical application. But carbon nanocones (CNCs) have drawn full attention after the discovery of free-standing structures or canonical topology as cap on one end of nanotubes (CNTs) [10–12]. CNCs are admired as alternatives of (CNTs) because of the absence of potentially poisonous metal catalyst in synthesis and mass production at room temperature [13]. In general, during the declamation of CNTs, strong acids are used in order to close out metal catalysts. In this process, deficiency introduced with the hindrance of destructing the graphite structure. On the other hand, the useful applications and attractive properties of CNCs are easy to approach. The application of CNCs as drug delivery capsules [14] and gas storage devices increased their significance in modern era. Throughout the years, this subject has been developing unique scientific obsession with planar, curved, and wrapped nanoscale structures, such as graphene, fullerines, and nanotubes [15]. It has a strong technological interest just as their innovative structural, noticeable electronic and mechanical properties. Curved carbon structures are used to investigate growth and nucleation. Especially, pentagon presence in CNCs plays vital role [16]. The 60 declination defect was detected when the pentagon inserted in a graphite sheet. This is the key of CNCs formation with pentagon as tip apex which leads us to the existence of nanotubes with tip topology [17]. This type of defects in graphite networks were theoretically considered for the study of electronic states [18]. CNCs have free-standing structures with sharp edges as these properties have applications in technology and electronics [19, 20]. The basic cell unit of carbon nanocone-consisting benzene ring is shown in Figure 1(a), and two benzene rings having a common edge in naphthalene is shown in Figure 1(b).

A graphical representation of these cones shows conical shape with a cycle of specific length at its core with hexagonal layers around the core. We are interested particularly in a structure with some different structural forms with $n$ layers of hexagons around the centre. In Section 3, we will explain the nodal structural form derived from CNC very similar to the bow-tie shape. Javaid et al. discussed some important results related to rhombus-type silicate and oxide networks and calculated indices to study the chemical behaviour [21]. Chemical properties and chemical bonding networking in the neural network were studied significantly by using indices [22, 23]. These gave a wider range to study the connection numbers and other indices on different chemical networks for observing the chemical behaviour and connectivity among the chemical bonds. Calculation of Zagreb connection numbers is based upon the specific distance. Formulas for many topological indices look like similar to one another. Degree-based, distance-based, and specific-restricted domain topological indices can differentiate among all of them. Leap Zagreb indices, dominating topological indices, and zagreb connection indices are close to each other by formulas but different by chemical structural properties of chemical structural-based compound [24].

3. Hourglass Section in Carbon Nanocone

Carbon nanocones have nice and interesting geometrical properties. These structures are connected, with infinite chains of concatenated hexagons having the property of two adjacent connected hexagons with a common edge. The construction property defines a definite rule for carbon nanostructure and it provides building block structure. That is why, it gives a planar simple connected graph obtained by connected regular hexagons [25].

Observing this geometrical property of the CNC here, we will describe its structure as similar to the hourglass. In this system, the core is centred with a cycle of specific length, whereas the layers of hexagons are around it. Moreover, this structure is similar to the doubled cone having a common
cycle core at the centre. We will term this unique novel system as “hourglass system carbon nanocone” (HGSCNC), whereas we will express the n-dimensional system as HGSCNC(n,k), where n is the dimension of the system which is the number of hexagon layers around the core and k represent the length of cycle at the core. We will discuss two cases for k: (1) when k is odd and (2) when k is even.

3.1. When Length of Cycle m Is Odd in n-Dimensional HGSCNC. In this case, we are presenting the HGSCNC with a cycle of odd length m up to n-dimension. We will observe sharpness and scattered pattern in n-dimensional hexagonal layers with odd length cycle. By observing the structural property of this particular case, we have found that this structure has 2n^2 + 12n + m total number of vertices with n ≥ 2 and m ≥ 7, whereas the edge set has total 3n^2 + 15n + m edges with n ≥ 2 and m ≥ 9. Here, n represents the number of hexagon layers and m ∈ O is the length of the cycle. A simple connected graph for this particular case is shown in Figure 2 and mathematically expressed as HGSCNC(n,m). A graphical display for HGSCNC for n = 4 with cycle of odd length for m = 7 is shown in Figure 3.

By working on some structural properties and behaviour of HGSCNC(n,m) up to n dimensions, we found it very interesting and rapid growing network. Here, we will state a lemma about its structural behaviour given as follows.

\[
\begin{align*}
ZC_1 (HGSCNC(n,m)) &= 72n^2 + 192n + 4m + 30/n \geq 2 \text{ and } m \geq 7, \\
ZC_2 (HGSCNC(n,m)) &= 108n^2 + 228n + 4m + 40/n \geq 2 \text{ and } m \geq 9, \\
ZC_1^n (HGSCNC(n,m)) &= 36n^2 + 120n + 4m + 70/n \geq 2 \text{ and } m \geq 9.
\end{align*}
\]

**Proof.** Working on Lemma 1, we have found some properties of the vertex set in Table 1 and edge set properties in Table 2 concluded as a result of 2 for HGSCNC(n,m) depending on the connection number of carbon atoms in the n-dimensional network. By using equation (1), we have

\[
ZC_1 (HGSCNC(n,m)) = 4(m-3) + 9(10) + 16(12n - 10) + 25(2) + 36(2n^2 - 1) + 49(2)
\Rightarrow ZC_1 (HGSCNC(n,m)) = 72n^2 + 192n + 4m + 30.
\]

**Lemma 1.** For n ≥ 2 and m = 7 HGSCNC, we have the first Zagreb connection number ZC_1 which is as follows:

\[
ZC_1 (HGSCNC(n,7)) = 72n^2 + 192n + 58.
\]

**Lemma 2.** For n ≥ 2 and m = 9 HGSCNC, we have first Zagreb connection number ZC_1, second Zagreb connection number ZC_2, and first modified Zagreb connection number ZC_1^n which are as follows:

\[
\begin{align*}
ZC_1 (HGSCNC(n,9)) &= 108n^2 + 228n + 84, \\
ZC_1^n (HGSCNC(n,9)) &= 36n^2 + 120n + 46.
\end{align*}
\]

3.1.1. Main Results. In this section, we will state our main results about connection numbers with the help of the abovementioned lemma and its consequences. These results are related to Zagreb connection numbers HGSCNC(n,m).

**Theorem 1.** Hourglass carbon nanocone system holds closed expression for first Zagreb connection number ZC_1, second Zagreb connection number ZC_2, and first modified Zagreb connection number ZC_1^n which are as follows:

\[
\begin{align*}
ZC_1 (HGSCNC(n,m)) &= 72n^2 + 192n + 4m + 30/n \geq 2 \text{ and } m \geq 7, \\
ZC_2 (HGSCNC(n,m)) &= 108n^2 + 228n + 4m + 40/n \geq 2 \text{ and } m \geq 9, \\
ZC_1^n (HGSCNC(n,m)) &= 36n^2 + 120n + 4m + 70/n \geq 2 \text{ and } m \geq 9.
\end{align*}
\]
Figure 2: Generalized hourglass carbon nanocone HGSCNC\((n, m)\).

Figure 3: Hourglass carbon nanocone HGSCNC\((4, 7)\).

Table 1: Vertex partition of HGSCNC\((n, m)\) for \(n \geq 2\) and \(m \geq 7\) with respect to connection number \(\tau\).

| \(\tau_u\) | 2     | 3     | 4     | 5     | 6     | 7     |
|------------|-------|-------|-------|-------|-------|-------|
| Number of vertices | \(m - 3\) | 10    | 12n - 10 | 2     | 2n^2 - 1 | 2     |

Table 2: Edge partition of HGSCNC\((n, m)\) for \(n \geq 2\) and \(m \geq 9\).

| \((\tau_u, \tau_v)\) | (2, 3) | (4, 3) | (4, 4) | (4, 5) | (6, 6) | (4, 6) | (5, 6) | (6, 7) | (4, 7) | (2, 2) |
|----------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Number of edges      | 10    | 10    | 12n - 16 | 2     | 3n^2 - 3n - 2 | 6n - 4 | 2     | 4     | 2     | \(m - 8\) |
From equation (2) and by using the abovementioned connection numbers for different edges, we have

$$ZC_2(HGSCNC(n, m)) = 6(10) + 12(10) + 16(12n - 16) + 20(2) + 36(3n^2 - 3n - 2) + 24(6n - 4) + 30(2) + 42(4) + 28(2) + 4(m - 8) \quad (8)$$

$$\Rightarrow ZC_2(CNC_n(n)) = 108n^2 + 228n + 4m + 40.$$ 

From equation (3) and by using the abovementioned connection numbers for different edges, we have

$$ZC_1^*(HGSCNC(n, m)) = 5(10) + 7(10) + 8(12n - 16) + 9(2) + 12(3n^2 - 3n - 2) + 10(6n - 4) + 11(2) + 13(4) + 11(2) + 4(m - 8) \quad (9)$$

$$\Rightarrow ZC_1^*(HGSCNC(n, m)) = 36n^2 + 120n + 4m + 70.$$ 

3.2. When the Length of Cycle $p$ Is Even in $n$-Dimensional HGSCNC. In this case, we are presenting the HGSCNC with even length $p \in E$ cycle up to $n$ dimensions. We will observe sharpness and scattered pattern in $n$-dimensional hexagonal layers with even length cycle. On observing the structural property of this particular case, we have found that this structure has $2n^2 + 8n + p + 8$ total number of vertices with $n \geq 2$ and $p \geq 10$, whereas the edge set has total $3n^2 + 15n + p$ edges with $n \geq 2$ and $p \geq 14$. Here, $n$ is representing the number of hexagon layers and $p \in E$ is the length of cycle. A simple connected graph for this particular case is shown in Figure 4 and mathematically expressed as $HGSCNC(n, p)$. A graphical display for HGSCNC for $n = 3$ with a cycle of odd length for $p = 10$ is shown in Figure 5.

On working some structural properties and behaviour of $HGSCNC(n, m)$ up to $n$ dimensions, we found it very interesting and rapid growing network. Here, we will state some lemmas about particular cases for connection numbers when the length of the cycle is fixed.

**Lemma 3.** For $n \geq 2$ and $p = 10$ HGSCNC, we have first Zagreb connection number $ZC_1$ which is as follows:

$$ZC_1(HGSCNC(n, 10)) = 72n^2 + 128n + 156. \quad (10)$$

**Lemma 4.** For $n \geq 2$ and $p = 14$ HGSCNC, we have first Zagreb connection number $ZC_1$, second Zagreb connection number $ZC_2$, and first modified Zagreb connection number $ZC_1^*$ which are as follows:

$$ZC_1^*(HGSCNC(n, 14)) = 108n^2 + 228n + 32, \quad (11)$$

$$ZC_1(HGSCNC(n, 14)) = 72n^2 + 128n + 4p + 116, \quad (12)$$

$$\forall n \geq 2 \text{ and } p \geq 10$$

$$ZC_2(HGSCNC(n, p)) = 108n^2 + 228n + 4p - 24, \quad (13)$$

$$\forall n \geq 2 \text{ and } p \geq 14$$

$$ZC_1^*(HGSCNC(n, p)) = 36n^2 + 120n + 4p \forall n \geq 2 \text{ and } p \geq 14. \quad (14)$$

**Proof.** Working on the lemma, we have found some properties of the vertex set in Table 3 and edge set in Table 4 of HGSCNC($n$, $p$) depending on the connection number of carbon atoms in the $n$-dimensional network. By using equation (1), we have
From equation (2) and by using the abovementioned connection numbers for different edges, we have

\[ ZC_1(HGSCNC(n, p)) = 4(p - 6) + 9(12) + 16(8n + 2) + 36(2n^2) \]
\[ \Rightarrow ZC_1(HGSCNC(n, p)) = 72n^2 + 128n + 4p + 116. \]  

\[ ZC_2(HGSCNC(n, p)) = 6(12) + 12(12) + 16(12n - 12) + 36(3n^2 - 3n) + 24(6n) + 4(p - 12) \]
\[ \Rightarrow ZC_2(HGSCNC(n, p)) = 108n^2 + 228n + 4p - 24. \]
From equation (3) and by using the abovementioned connection numbers for different edges, we have

\[ ZC^*_1 \text{ (HGSCNC}(n, p)) = 5(12) + 7(12) + 8(12n - 12) + 12(3n^2 - 3n) + 10(6n) + 4(p - 12) \]

\[ \Rightarrow ZC^*_1 \text{ (HGSCNC}(n, p)) = 36n^2 + 120n + 4p. \]

4. Graphical Comparison

In this section, we will compare our results via graphical view. Firstly, we have compared our output results among \( ZC_1 \), \( ZC_2 \), and \( ZC^*_1 \) for HGSCNC \((n, m)\), and results are shown in Figure 6(a). Similarly, we have compared our output results among \( ZC_1 \), \( ZC_2 \), and \( ZC^*_1 \) for HGSCNC \((n, p)\), and results are shown in Figure 6(b).

5. Conclusion

In this article, we have computed closed results for the family of Zagreb connection number in the hourglass system carbon nanocone (HGSCNC) and with its core of even length and its core of odd length. For the first time, we have evaluated the Zagreb connection numbers for HGSCNC \((n, m)\) and HGSCNC \((n, p)\). The results are very interesting, and we concluded that HGSCNC \((n, m)\) is the fast predicting network as compared to HGSCNC \((n, p)\). Furthermore, we have concluded that \( ZC_2 \) has better prediction for both HGSCNC \((n, m)\) as well as for HGSCNC \((n, p)\). Predicting ability of a topological index encourages the theoretical study of the chemical structure. We computed Zagreb connection indices \( ZC_1, ZC_2, \) and \( ZC^*_1 \) for HGSCNC up to \( n \) dimensions for different lengths of central core. These results will facilitate the understanding of
topological properties of the noval structure of HGSCNC. Our results will motivate to investigate new structure of different chemical structures and their line graphs and studying their topological and physical properties.

Data Availability
No data were used to support this study.

Disclosure
The paper has not been published elsewhere, and it will not be submitted anywhere else for publication.

Conflicts of Interest
The authors declare no conflicts of interest.

Authors’ Contributions
All authors contributed equally to this work.

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