Research Article

Study of Carbon Nanocones $CNC_k(n)$ via Connection Zagreb Indices

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Topology of fullerenes, carbon nanotubes, and nanocones has considerable worth due to their effective applications in nanotechnology. These are emerging materials of practical application in gas storage devices, nanoelectronics devices, energy storage, biosensor, and chemical probes. The topological indices are graph invariant used to investigate the physical and chemical properties of the compounds such as boiling point, stability, and strain energy through associated chemical graph of the underlying compound. We computed recently modified Zagreb connection indices of nanocones $CNC_4(n)$, $CNC_5(n)$, and $CNC_6(n)$ and generalized our findings up to a large class of $CNC_k(n)$. Topological characterization of nanocones via these indices is mathematically novel and assists to enable its emerging use in nanotechnology. For computation and verification of results, we use Mathematica software.

1. Introduction

Carbon nanomaterials received considerable attention due to their effective physical applications in nanotechnology [1] as emerging materials of practical application. However, carbon nanocones (CNCs) received considerable attention after the discovery of free-standing structures or canonical topology as cap on one end of nanotubes (CNTs) [2, 3]. CNCs are considered as alternatives of (CNTs) due to the absence of potentially poisonous metal catalyst in synthesis and mass production at room temperature [4]. Generally, during the declamation of CNTs, strong acids are used in

order to close out metal catalysts. In this process, deficiency is introduced with the hindrance of destructing the graphite structure. On the contrary, the applications and properties of CNCs are easy to approach. CNCs' application as drug delivery capsules [5] and gas storage devices increased their significance. Throughout the years, this subject has been developing scientific obsession with planar, curved, and wrapped nanoscale structures, such as graphene, fullerenes, and nanotubes. It has a strong technological interest just because of their innovative structural, electronic, and mechanical properties. Curved carbon structures are used to investigate growth and nucleation. Especially, pentagon

presence in CNCs plays a vital role [6]. The 60 declination defect is detected when pentagon inserted in the 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. This type of defects in graphite networks is theoretically considered for study of electronic states [7]. CNCs have free-standing structures with sharp edges because these properties have applications in technology and electronics [8]. In Figure 1, the canonical form of CNCs is shown in Figure 1(a) and associated chemical graph is shown in Figure 1(b). We are interested in the characterization of CNCs using chemical graph theory.

1.1. Graph. Let $G = (V, E)$ be a graph comprising set of vertices V and $E \subseteq \binom{V}{2}$ as the set of edges. A graph is called the directed graph if the edges have some orientations. In a multigraph, two vertices can share more than one edge. A loop in a graph is an edge joining a vertex to itself. Graph is called simple if it is not directed or multigraph and has no loops.

1.2. Chemical Graph Theory. Graph theory is considered as a powerful tool in different areas of research such as in coding theory, database management system, circuit design, secret sharing schemes, and theoretical chemistry. Chemical graph theory is the combination of chemistry and graph theory. It develops a relationship between structure of organic substances and their physio-chemical properties through some useful graph invariants with the help of their associated molecular graph. The molecular graph is a simple graph on vertices which are representatives of atoms of corresponding chemical substance and edges placed against the bonds between atoms. Figure 2 depicts chemical graphs of some hydrocarbons as benzene in Figure 2(a) and naphthalene in Figure 2(b). The theoretical study of underlying substance using molecular graphs through graph invariants has effective applications in quantitative structure properties relationship (QSPR) or quantitative structure activities relationship (QSAR) investigation [9].

2. Topological Indices

Topological indices among graph invariants have a special place and are used to estimate the physio-chemical properties of chemical compound. A topological index is considered as a function $f: G \rightarrow R$ which maps each graph of chemical structures into a numerical value and have special place among other graph invariants due to its estimation applicability for physio-chemical properties of chemical compound. The idea of topological indices was first introduced by Wiener in 1947 during the work on paraffin's boiling points [10]. In 1972, Zagreb indices were introduced by Ivan Gutman and Trinajstić [11]. Second Zagreb index was thought of by Hosoya et al. in 1975 [12]. The first and second Zagreb indices are defined as

$$\begin{aligned} M_1(\Gamma) &= \sum_{uv \in E(\Gamma)} (\deg_u + \deg_v), \\ M_2(\Gamma) &= \sum_{uv \in E(\Gamma)} (\deg_u \times \deg_v). \end{aligned} \quad (1)$$

Recently, modified versions of Zagreb indices were introduced and studied independently in [13–15]. These indices based on connection number are assigned to the vertices of graph. For more detail of topological indices, one can refer to [16–18].

2.1. Connection Number. Let G be a graph. The connection number associated to the vertex $u \in V(G)$ is the number of distinct vertices at distance two from vertex u . It is denoted by τ_u :

$$\tau_u = |\{v \in V(G) : d(u, v) = 2\}|. \quad (2)$$

2.2. Connection Zagreb Indices. The first $ZC_1(G)$ and second $ZC_2(G)$ connection Zagreb indices are defined as

$$\begin{aligned} ZC_1(G) &= \sum_{u \in V(G)} \tau_u^2, \\ ZC_2(G) &= \sum_{uv \in E(G)} \tau_u \times \tau_v, \end{aligned} \quad (3)$$

where ZC_1^* is another recently introduced graph invariant over connection number [19]:

$$ZC_1^*(G) = \sum_{u \in V(G)} (\deg_u \tau_u) = \sum_{uv \in E(G)} (\tau_u + \tau_v), \quad (4)$$

where $\deg_u$ stands for degree of $u \in (G)$ and τ_u is the connection number assigned to u . Ali et al. [19] proved that, for triangle and rectangle free graphs, connection number τ_u assigned to a vertex u is $\tau_u = \sum_{uv \in E(G)} \deg_v - \deg_u$.

2.3. Applications of Connection Zagreb Indices in Chemistry. Applicability of $ZC_1(G)$, $ZC_2(G)$, and $ZC_1^*(G)$ is observed by its good correlation with entropy of octane isomers [19]. Ali et al. [20] concluded that ZC_1^* has correlation coefficient approximately 0.949 and 0.892 for acentric factor and entropy, respectively, and ZC_1 has a good correlation with enthalpy. Javaid et al. studied T-sum graphs and graphs constructed through graph operation using connection indices [21–25]. This contemplation recommends chemical applicability of these indices as useful descriptor in QSAR and QSPR investigation.

3. Materials and Methods

In this work, we use graph theoretic techniques adopted in [21–25] to study the topology of the corresponding molecular graph of underlying compound for their insight investigation. We used investigative procedure, vertex segment strategy, edge segment procedure, and degree tallying strategy along with combinatorial enlisting techniques, number theoretic logics, and edges and vertices partition

FIGURE 1: Carbon nanocones with associated chemical graph. (a) Canonical form of carbon nanocones. (b) Chemical Graph of carbon nanocones.

FIGURE 2: Some hydrocarbons with associated chemical graphs. (a) Benzene with chemical graph. (b) Naphthalene with chemical graph.

according to the values associated to the vertices for desired computation.

Throughout this work, we use standard graph theoretic notations, graph $G = (V, E)$, set of vertices $V(G)$ and the set of edges $E(G)$ of a graph G with $|V|$ order and $|E|$ size of G , $\deg_{v_i}$ as degree for vertex v_i , and the number of edges incident to v_i . We draw graph of $\text{CNC}_k(n)$ using Mathematica software for $k = 4, 5, 6$ and compute degree sequence for different values of n . Through observations, we listed possibilities for connection numbers assigned to the vertices and determined vertex petition as well as edge partitions with respect to connection number assigned to the vertices of these graphs.

4. Results and Discussion

In this work, we compute connection Zagreb indices $ZC_1(G)$, $ZC_2(G)$, and $ZC_1^*(G)$ of CNCs which are helpful in their topological investigation and generalize our findings up to a large class of $\text{CNC}_k(n)$. $\text{CNC}_k(n)$ are classified on the basis of k , where k is the number of carbon atoms present in

the core of nanocones and n is the number of hexagon layers around the core [26].

4.1. Results for $\text{CNC}_4(n)$. In [27], Ghorbani and Jalali compute vertex PI index, Szeged index, and Omega Polynomials, and Hayat and Imran [28] computed ABC_4 and GA_5 of $\text{CNC}_4(n)$. In Theorem 1, we computed connection Zagreb indices of $\text{CNC}_4(n)$. $\text{CNC}_4(n)$ for $n = 3$ is shown in Figure 3.

Theorem 1. The ZC_1, ZC_2 , and ZC_1^* of $\text{CNC}_4(n)$ are

$$\begin{aligned} ZC_1(\text{CNC}_4(n)) &= 144n^2 + 128n + 8, \\ ZC_2(\text{CNC}_4(n)) &= 216n^2 + 152n + 4, \\ ZC_1^*(\text{CNC}_4(n)) &= 72n^2 + 80n + 16. \end{aligned} \quad (5)$$

Proof. Let $G = \text{CNC}_4(n)$ be the graph of under consideration CNCs. The total number of vertices of $\text{CNC}_4(n)$ are $4(n+1)^2$ and $2(3n^2 + 5n + 2)$ edges. We made partition of

FIGURE 3: $\text{CNC}_4(3)$.

vertex set with respect to the connection number τ_u as $V_{\tau_u}(G)$. For this purpose, we draw graphs of $\text{CNC}_4(n)$ for $n = 1, 2, 3$ using Mathematica and compute degree sequence as $\{2, 3\}$. Degree sequence $\{2, 3\}$ of $\text{CNC}_4(n)$ implies 3, 4, and 6 are the only possibilities of the connection numbers associated to the vertices of G and $(3, 3)$, $(3, 4)$, $(4, 4)$, $(4, 6)$, and $(6, 6)$ are the possibilities for the edges. For partition of edges having the same end vertices connection numbers, we use edge and vertex segment strategy along with edges and vertex listing technique. The following tabular calculation enables us for this partition through induction.

The numerical results of Table 1 depict $|V_3(G)| = 8$, $|V_4(G)| = 8n - 4$, and $|V_6(G)| = 4n^2$. By using this partition, we computed $\text{ZC}_1(\text{CNC}_4(n))$:

$$\text{ZC}_1(G) = \sum_{u \in V(G)} \tau_u^2. \quad (6)$$

Let $N_\tau = \{\tau_u : u \in V(G)\}$, and from vertex partition $V_{\tau_u}(G)$, we obtain

$$\begin{aligned} \text{ZC}_1(G) &= \sum_{\tau_u \in N_\tau} \sum_{u \in V_{\tau_u}(G)} \tau_u = \sum_{u \in V_3(G)} \tau_u + \sum_{u \in V_4(G)} \tau_u + \sum_{u \in V_6(G)} \tau_u, \\ \text{ZC}_1(G) &= 8(3)^2 + (8n - 4)(4)^2 + 4n^2(6)^2, \\ \text{ZC}_1(\text{CNC}_4(n)) &= 144n^2 + 16(8n - 4) + 72. \end{aligned} \quad (7)$$

In Table 2, we list our observation for the number of edges with similar end vertex connection number and generalize our findings for arbitrary value of n .

The generalization based on Table 2 provides edge partitions as $E_{(\tau_u, \tau_v)}(G)$: $|E_{(3,3)}(G)| = 4$, $|E_{(3,4)}(G)| = 8$, $|E_{(4,4)}(G)| = 8(n - 1)$, $|E_{(4,6)}(G)| = 4n$, and $|E_{(6,6)}(G)| = 2n$

$(3n - 1)$. Using this partition, we computed $\text{ZC}_2(\text{CNC}_k(n))$ defined as

$$\text{ZC}_2(G) = \sum_{uv \in E(G)} \tau_u \tau_v. \quad (8)$$

Let $M_\tau = \{(\tau_u, \tau_v) : uv \in G\}$:

$$\begin{aligned}
ZC_2(G) &= \sum_{(\tau_u, \tau_v) \in M_\tau} \sum_{uv \in E_{(\tau_u, \tau_v)}(G)} \tau_u \tau_v = \sum_{uv \in E_{(3,3)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(3,4)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(4,4)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(4,6)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(6,6)}(G)} \tau_u \tau_v, \\
ZC_2(G) &= 4(3 \times 3) + 8(3 \times 4) + (8n - 8)(4 \times 4) + 4n(4 \times 6) + 2n(3n - 1)(6 \times 6), \\
ZC_2(G) &= 216n^2 + 152n + 4.
\end{aligned} \tag{9}$$

Now, we compute $ZC_1^*(G)$ which is defined as

$$ZC_1^*(G) = \sum_{u \in V(G)} \tau_u \deg_u = \sum_{uv \in E_{(u,v)}(G)} (\tau_u + \tau_v). \tag{10}$$

Let $O_\tau = \{(\tau_u, \tau_v): uv \in E(G)\}$ and

$$\begin{aligned}
ZC_1^*(G) &= \sum_{(\tau_u, \tau_v) \in O_\tau} \sum_{uv \in E_{(\tau_u, \tau_v)}(G)} (\tau_u + \tau_v) = \sum_{uv \in E_{(3,3)}(G)} (\tau_u + \tau_v) + \sum_{uv \in E_{(3,4)}(G)} (\tau_u + \tau_v) + \sum_{uv \in E_{(4,4)}(G)} (\tau_u + \tau_v) \\
&\quad + \sum_{uv \in E_{(4,6)}(G)} (\tau_u + \tau_v) + \sum_{uv \in E_{(6,6)}(G)} (\tau_u + \tau_v), s,
\end{aligned} \tag{11}$$

$$ZC_1^*(G) = 4(3 + 3) + 8(3 + 4) + (8n - 8)(4 + 4) + 4n(4 + 6) + 2n(3n - 1)(6 + 6),$$

$$ZC_1^*(G) = 72n^2 + 80n + 16.$$

4.2. Results for $CNC_5(n)$. A. R. Ashrafi in [29] computed winner index of $CNC_5(n)$. In Theorem 2, we computed connection Zagreb indices of $CNC_5(n)$ whose chemical graph for $n = 3$ is shown in Figure 4.

Theorem 2. The ZC_1, ZC_2 , and ZC_1^* of $CNC_5(n)$ are equal to

$$\begin{aligned}
ZC_1(CNC_5(n)) &= 180n^2 + 160n + 10, \\
ZC_2(CNC_5(n)) &= 270n^2 + 190n + 5, \\
ZC_1^*(CNC_5(n)) &= 90n^2 + 100n + 20.
\end{aligned} \tag{12}$$

Proof. The total number of vertices of $G = CNC_5(n)$ are $5(n + 1)^2$ and edges $5/2(3n^2 + 5n + 2)$. Like $CNC_4(n)$, we partitioned the vertex set as $V_{\tau_u}(G)$ and the edge set as $E_{(\tau_u, \tau_v)}(G)$ by using edge and vertex segment strategy along with edges and vertex listing technique for desired partition.

The computations in Table 3 depict $|V_3(G)| = 10$, $|V_4(G)| = 10n - 5$, and $|V_6(G)| = 5n^2$. By using this partition, we compute $ZC_1(CNC_5(n)) = ZC_1(G)$ as

$$ZC_1(G) = \sum_{u \in V(G)} \tau_u^2. \tag{13}$$

Let $N_\tau = \{\tau_u: u \in V(G)\}$; then, by using vertex set partition $V(\tau_u)$, we obtain

$$\begin{aligned}
ZC_1(G) &= \sum_{\tau_u \in N_\tau} \sum_{u \in V_{\tau_u}(G)} \tau_u = \sum_{u \in V_3(G)} \tau_u + \sum_{u \in V_4(G)} \tau_u + \sum_{u \in V_6(G)} \tau_u, \\
ZC_1(G) &= 10(3)^2 + (10n - 5)(4)^2 + 5n^2(6)^2, \\
ZC_1(CNC_5(n)) &= 180n^2 + 160n + 10.
\end{aligned} \tag{14}$$

In Table 4, we list our observation for the number of edges with similar end vertex connection number and generalize our findings for n .

The generalization based on Table 4 provides edge partitions as $E_{(\tau_u, \tau_v)}(G): |E_{(3,3)}(G)| = 5, |E_{(3,4)}(G)| = 10, |E_{(4,4)}(G)| = 10(n - 1), |E_{(4,6)}(G)| = 5n$, and $|E_{(6,6)}(G)| = 5n^2$.

TABLE 1: Vertex partition of $CNC_4(n)$ with respect to connection number τ .

n	1	2	3	4	5	6	7	8	9	10	...	p
$\tau_u = 3$	8	8	8	8	8	8	8	8	8	8	...	8
$\tau_u = 4$	4	12	20	28	38	44	52	60	68	76	...	$8p - 4$
$\tau_u = 6$	4	16	36	64	100	144	196	256	324	400	...	$4p^2$

TABLE 2: Edge partition of $CNC_4(n)$ with respect to connection number τ .

$n/ E_{(\tau_u, \tau_v)} $	1	2	3	4	5	6	7	8	9	10	...	$n = p$
$ E_{(3,3)} $	4	4	4	4	4	4	4	4	4	4	...	4
$ E_{(3,4)} $	8	8	8	8	8	8	8	8	8	8	...	8
$ E_{(4,4)} $	0	8	16	24	32	40	48	56	64	72	...	$8(p-1)$
$ E_{(4,6)} $	4	8	12	16	20	24	28	32	36	40	...	$4p$
$ E_{(6,6)} $	4	20	48	88	140	204	280	368	468	580	...	$2p(3p-1)$

FIGURE 4: Chemical graph of $CNC_5(n)$ for $n = 3$.TABLE 3: Vertex partition of $CNC_5(n)$ with respect to connection number τ .

n	1	2	3	4	5	6	7	8	9	10	...	p
$\tau = 3$	10	10	10	10	10	10	10	10	10	10	...	10
$\tau = 4$	5	15	25	35	45	55	65	75	85	95	...	$10p - 5$
$\tau = 6$	5	20	45	80	125	180	245	320	405	500	...	$5p^2$

TABLE 4: Edge partition of $CNC_5(n)$ with respect to connection number τ .

$n/ E_{(\tau_u, \tau_v)} $	1	2	3	4	5	6	7	8	9	10	...	$n = p$
$ E_{(3,3)} $	5	5	5	5	5	5	5	5	5	5	...	5
$ E_{(3,4)} $	10	10	10	10	10	10	10	10	10	10	...	10
$ E_{(4,4)} $	0	10	20	30	40	50	60	70	80	90	...	$10(p-1)$
$ E_{(4,6)} $	5	10	15	20	25	30	35	40	45	50	...	$5p$
$ E_{(6,6)} $	5	25	60	110	175	255	350	460	585	725	...	$5p/2(3p-1)$

$|G| = 5/2n(3n - 1)$. Using this partition, we computed ZC_2 ($CNC_5(n)$) and ZC_1^* ($CNC_5(n)$):

$$ZC_2(G) = \sum_{uv \in E(G)} \tau_u \tau_v. \quad (15)$$

Let $M_\tau = \{(\tau_u, \tau_v): uv \in G\}$; then, by using vertex edge partition $E_{(\tau_u, \tau_v)}(G)$, we obtain

$$\begin{aligned} ZC_2(G) &= \sum_{(\tau_u, \tau_v) \in M_\tau} \sum_{uv \in E_{(\tau_u, \tau_v)}(G)} \tau_u \tau_v = \sum_{uv \in E_{(3,3)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(3,4)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(4,4)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(4,6)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(6,6)}(G)} \tau_u \tau_v \\ &= 5(3 \times 3) + 10(3 \times 4) + (10n - 10)(4 \times 4) + 5n(4 \times 6) + 5/2n(3n - 1)(6 \times 6) \\ &= 270n^2 + 190n + 5. \end{aligned} \quad (16)$$

For $ZC_1^*(G)$,

$$ZC_1^*(G) = \sum_{u \in V(G)} \tau_u \deg_u = \sum_{uv \in E_{(u,v)}(G)} (\tau_u + \tau_v). \quad (17)$$

Let $O_\tau = \{(\tau_u, \tau_v): uv \in E(G)\}$:

$$\begin{aligned} ZC_1^*(G) &= \sum_{(\tau_u, \tau_v) \in O_\tau} \sum_{uv \in E_{(\tau_u, \tau_v)}(G)} (\tau_u + \tau_v) = \sum_{uv \in E_{(3,3)}(G)} (\tau_u + \tau_v) + \sum_{uv \in E_{(3,4)}(G)} (\tau_u + \tau_v) + \sum_{uv \in E_{(4,4)}(G)} (\tau_u + \tau_v) \\ &\quad + \sum_{uv \in E_{(4,6)}(G)} (\tau_u + \tau_v) + \sum_{uv \in E_{(6,6)}(G)} (\tau_u + \tau_v) \\ &= 5(3 + 3) + 10(3 + 4) + (10n - 10)(4 + 4) + 5n(4 + 6) + \frac{5}{2}n(3n - 1)(6 + 6) = 90n^2 + 100n + 20. \end{aligned} \quad (18)$$

4.3. Results for $CNC_6(n)$. In Theorem 3, we computed connection Zagreb indices of $CNC_k(n)$, for $k = 6$. $CNC_6(n)$ for $n = 4$ is shown in Figure 5.

Theorem 3. The ZC_1, ZC_2 , and ZC_1^* of $CNC_5(n)$ are equal to

$$\begin{aligned} ZC_1(CNC_6(n)) &= 180n^2 + 160n + 10, \\ ZC_2(CNC_6(n)) &= 270n^2 + 190n + 5, \\ ZC_1^*(CNC_6(n)) &= 108n^2 + 100n + 20. \end{aligned} \quad (19)$$

Proof. The total number of vertices of $G = CNC_6(n)$ are $6(n + 1)^2$ and $3(3n^2 + 5n + 2)$ edges. Similar technique is

used as in $CNC_4(n)$ and $CNC_5(n)$ computation. We partitioned the vertex set as $V_{\tau_u}(G)$ and the edge set as $E_{(\tau_u, \tau_v)}(G)$.

The computations in Table 5 give vertex partition $|V_3(G)| = 10, |V_4(G)| = 10n - 5$, and $|V_6(G)| = 5n^2$. By using this partition, we compute $ZC_1(CNC_6(n)) = ZC_1(G)$:

$$ZC_1(G) = \sum_{u \in V(G)} \tau_u^2. \quad (20)$$

Let $N_\tau = \{\tau_u: u \in V(G)\}$:

$$\begin{aligned} ZC_1(G) &= \sum_{\tau_u \in N_\tau} \sum_{u \in V_{\tau_u}(G)} \tau_u = \sum_{u \in V_3(G)} \tau_u + \sum_{u \in V_4(G)} \tau_u + \sum_{u \in V_6(G)} \tau_u, \\ ZC_1(G) &= 12(3)^2 + (12n - 6)(4)^2 + 6n^2(6)^2, \\ ZC_1(CNC_6(n)) &= 216n^2 + 192n + 12. \end{aligned} \quad (21)$$

In Table 6, we list our observation for the number of edges with similar end vertex connection number of $CNC_6(n)$ and generalize for arbitrary value of n .

The generalization based on Table 6 provides edge partitions as $E_{(\tau_u, \tau_v)}(G), |E_{(3,3)}(G)| = 6, |E_{(3,4)}(G)| = 12, |E_{(4,4)}(G)| = 12(n - 1), |E_{(4,6)}(G)| = 6n$, and $|E_{(6,6)}(G)|$

FIGURE 5: Graphical representation of $\text{CNC}_6(n)$.

$= 3n(3n - 1)$. Using this partition, we computed $\text{ZC}_2(\text{CNC}_6(n))$ and $\text{ZC}_1^*(\text{CNC}_6(n))$:

Let $M_\tau = \{(\tau_u, \tau_v) : uv \in G\}$,

$$\text{ZC}_2(G) = \sum_{uv \in E(G)} \tau_u \tau_v, \quad (22)$$

$$\begin{aligned} \text{ZC}_2(G) &= \sum_{(\tau_u, \tau_v) \in M_\tau} \sum_{uv \in E_{(\tau_u, \tau_v)}(G)} \tau_u \tau_v = \sum_{uv \in E_{(3,3)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(3,4)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(4,4)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(4,6)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(6,6)}(G)} \tau_u \tau_v \\ &= 6(3 \times 3) + 12(3 \times 4) + (12n - 12)(4 \times 4) + 6n(4 \times 6) + 3n(3n - 1)(6 \times 6), \end{aligned} \quad (23)$$

$$\text{ZC}_2(\text{CNC}_6(n)) = 324n^2 + 228n + 6.$$

Now, for $\text{ZC}_1^*(G)$,

Let $O_\tau = \{(\tau_u, \tau_v) : uv \in E(G)\}$:

$$\text{ZC}_1^*(G) = \sum_{u \in V(G)} \tau_u \deg_u = \sum_{uv \in E_{(u,v)}(G)} (\tau_u + \tau_v). \quad (24)$$

$$\begin{aligned} \text{ZC}_*^*(G) &= \sum_{(\tau_u, \tau_v) \in O_\tau} \sum_{uv \in E_{(\tau_u, \tau_v)}(G)} (\tau_u + \tau_v) = \sum_{uv \in E_{(3,3)}(G)} (\tau_u + \tau_v) + \sum_{uv \in E_{(3,4)}(G)} (\tau_u + \tau_v) + \sum_{uv \in E_{(4,4)}(G)} (\tau_u + \tau_v) \\ &\quad + \sum_{uv \in E_{(4,6)}(G)} (\tau_u + \tau_v) + \sum_{uv \in E_{(6,6)}(G)} (\tau_u + \tau_v) \\ &= 6(3 + 3) + 12(3 + 4) + (12n - 12)(4 + 4) + 6n(4 + 6) + 3n(3n - 1)(6 + 6), \end{aligned} \quad (25)$$

$$\text{ZC}_1^*(\text{CNC}_6(n)) = 108n^2 + 192n + 24.$$

□

TABLE 5: Vertex partition of $CNC_6(n)$ with respect to connection number τ .

n	1	2	3	4	5	6	7	8	9	10	...	p
$\tau = 3$	12	12	12	12	12	12	12	12	12	12	...	12
$\tau = 4$	6	18	30	42	54	66	78	90	102	114	...	$12p - 6$
$\tau = 6$	5	24	54	96	150	216	294	384	486	600	...	$6p^2$

TABLE 6: Edge partition of $CNC_6(n)$ with respect to connection number τ .

$n/ E_{(\tau_u, \tau_v)} $	1	2	3	4	5	6	7	8	9	10	...	$n = p$
$ E_{(3,3)} $	6	6	6	6	6	6	6	6	6	6	...	6
$ E_{(3,4)} $	12	12	12	12	12	12	12	12	12	12	...	12
$ E_{(4,4)} $	0	12	24	36	48	60	72	84	96	108	...	$12(p-1)$
$ E_{(4,6)} $	6	12	18	24	30	36	42	48	54	60	...	$6p$
$ E_{(6,6)} $	6	30	72	132	210	306	420	552	702	870	...	$3p(3p-1)$

FIGURE 6: Comparison of results computed in Theorems 1–3. (a) Comparison of results regarding ZC_1 . (b) Comparison of results regarding ZC_2 . (c) Comparison of results regarding ZC_1^* .

FIGURE 7: The chemical graph of generalized carbon nanocone $\text{CNC}_k(n)$.

FIGURE 8: The graphical representation of connection Zagreb indices for generalized values of n and k . (a) The graphical representation of $ZC_1(\text{CNC}_k(n))$. (b) The graphical representation of $ZC_2(\text{CNC}_k(n))$.

4.4. Comparison of Results. In Figure 6, Figure 6(a) interprets behavior of $ZC_1(G)$, Figure 6(b) of $ZC_2(G)$, and Figure 6(c) of $ZC_1^*(G)$ for $k = 4, 5, 6$.

4.5. Results for $\text{CNC}_k(n)$. Graph shown in Figure 7 is the associated chemical graph of $\text{CNC}_k(n)$ for arbitrary value of k . It consists of a k -gon as the central core cycle with n layers of hexagons around the core.

Theorem 4. The ZC_1, ZC_2 , and ZC_1^* of $\text{CNC}_k(n)$ are

$$\begin{aligned} ZC_1(\text{CNC}_k(n)) &= 36kn^2 + 32kn + 2k, \\ ZC_2(\text{CNC}_k(n)) &= 54kn^2 + 38kn + k, \\ ZC_1^*(\text{CNC}_k(n)) &= 18kn^2 + 20kn + 4k. \end{aligned} \quad (26)$$

Proof. The chemical graph of $\text{CNC}_k(n)$ has cycle of length k corresponding to core of $\text{CNC}_k(n)$, where n represent the number of layers of hexagons around the core. Total vertices of $\text{CNC}_k(n)$ is $k(n+1)^2$ and edges is $k/2(3n^2 + 5n + 2)$ [30].

FIGURE 9: The graphical representation of $ZC_1^*(CNC_k(n))$ for generalized values k .

For computation of ZC_1 for generalized nanocone $CNC_k(n)$, we used their edges and vertex partition. From the construction of $CNC_k(n)$, it is clear that the connection number associated to the vertices is 6 except the $k(2n+1)$ vertices of outer layer of hexagons. So, the number of vertices with connection number 6 is $|V_6(CNC_k(n))| = k(n+1)^2 - k(2n+1) = kn^2 = kn^2$.

In the outer layer of hexagons, two vertices at each corner have connection number $\tau_u = 3$ and all other have $\tau_u = 4$. So, $|V_3(CNC_k(n))| = 2k$ and $|V_4(CNC_k(n))| =$

$k(2n+1) - 2k = k(2n-1)$. Similarly, all the edges other than edges of the outer layer of hexagons have (6,6) as end vertex connection number, i.e., $|E_{(6,6)}(CNC_k(n))| = k/2(3n^2 + 5n + 2) - (3kn + k) = k/2(3n^2 - 1)$. The edges in the outer layer of hexagons are partitioned as $|E_{(3,3)}(CNC_k(n))| = k$, $|E_{(3,4)}(CNC_k(n))| = 2k$, $|E_{(4,4)}(CNC_k(n))| = k(2n-2)$, and $|E_{(4,6)}(CNC_k(n))| = kn$. We use this vertex and edge partition and technique as used in Theorems 1–3 for proof. Let $G = CNC_K(n)$ and $N_\tau = \{\tau_u : u \in V(G)\}$:

$$ZC_1(G) = \sum_{u \in V(G)} \tau_u^2,$$

$$ZC_1(G) = \sum_{\tau_u \in N_\tau} \sum_{u \in V_{\tau_u}(G)} \tau_u = \sum_{u \in V_3(G)} \tau_u + \sum_{u \in V_4(G)} \tau_u + \sum_{u \in V_6(G)} \tau_u, \quad (27)$$

$$ZC_1(G) = 2k(3)^2 + k(2n-1)(4)^2 + kn^2(6)^2,$$

$$ZC_1(CNC_k(n)) = 36kn^2 + 32kn + 2k,$$

$$ZC_2(G) = \sum_{uv \in E(G)} \tau_u \tau_v,$$

$$ZC_2(G) = \sum_{(\tau_u, \tau_v) \in M_\tau} \sum_{uv \in E_{(\tau_u, \tau_v)}(G)} \tau_u \tau_v = \sum_{uv \in E_{(3,3)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(3,4)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(4,4)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(4,6)}(G)} \tau_u \tau_v + \sum_{uv \in E_{(6,6)}(G)} \tau_u \tau_v,$$

$$ZC_2(G) = k(3 \times 3) + 2k(3 \times 4) + (2kn - 2k)(4 \times 4) + kn(4 \times 6) + \frac{k}{2}(3n^2 - 1)(6 \times 6),$$

$$ZC_1(CNC_k(n)) = 54kn^2 + 38kn + k,$$

(28)

$$\begin{aligned}
ZC_1^*(G) &= \sum_{u \in V(G)} \tau_u \deg_u = \sum_{uv \in E_{(u,v)}(G)} (\tau_u + \tau_v), \\
ZC_1^*(G) &= \sum_{(\tau_u, \tau_v) \in O_\tau} \sum_{uv \in E_{(\tau_u, \tau_v)}(G)} (\tau_u + \tau_v) = \sum_{uv \in E_{(3,3)}(G)} (\tau_u + \tau_v) + \sum_{uv \in E_{(3,4)}(G)} (\tau_u + \tau_v) + \sum_{uv \in E_{(4,4)}(G)} (\tau_u + \tau_v) \\
&\quad + \sum_{uv \in E_{(4,6)}(G)} (\tau_u + \tau_v) + \sum_{uv \in E_{(6,6)}(G)} (\tau_u + \tau_v),
\end{aligned} \tag{29}$$

$$ZC_1^*(G) = k(3+3) + 2k(3+4) + (2kn-2k)(4+4) + kn(4+6) + \frac{k}{2}(3n^2-1)(6+6),$$

$$ZC_1^*(CNC_k(n)) = 18kn^2 + 20kn + 4k.$$

Hence, the proof is completed.

Theorem 4 shows that connection Zagreb indices of $CNC_k(n)$ increased by a factor k (number of carbon atoms in the core). In Figure 8, Figures 8(a) and 8(b) interpret computed results of $ZC_1(CNC_k(n))$ and $ZC_2(CNC_k(n))$, respectively, for any value of k and 9 of $ZC_1^*(CNC_k(n))$. $\square$

5. Conclusion

The International Academy of Theoretical Chemistry explored that any topological index is acceptable to estimate chemical properties of compounds if it has a sound correlation with actual physio-chemical property of octane isomers. Customarily, octane isomers are adopted for such investigations due to the huge number of structural isomers of octane [31] for the acceptable statistical conclusion. Ali et al. [32] studied the correlation efficiency of ZC_1^* for the physio-chemical properties of octane isomers: entropy, boiling point, density, enthalpies, acentric factor, etc. They concluded that ZC_1^* has a correlation coefficient approximately 0.949 and 0.892 for acentric factor and entropy, respectively. Correlation of ZC_1 with physical properties was studied by Jakkanavar and Basavanagoud [33] and found good with enthalpy. Possibility of large-scale production of CNCs [34] and predictive ability of topological indices [35] encourages theoretical study of $CNC_k(n)$. We computed connection Zagreb indices $ZC_1(G)$, $ZC_2(G)$, and $ZC_1^*(G)$ of $CNC_k(n)$ for $k = 4, 5, 6$ in Theorems 1–3 and generalized our finding up to large value of K in 4.4. These results facilitate topological characterization of $CNC_k(n)$ which is helpful in finding new applications in the emerging field of nanotechnology.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors of this paper declare that they have no conflicts of interest.

Authors' Contributions

All authors have contributed equally.

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