ON THE GENERAL RANDIC, SUM-CONNECTIVITY AND MODIFY RANDIC INDICES OF CARBON NANOCONES $CNC_k[n]$

by Jia-Bao Liu[1], Muhammad K. Jamil[2], Mohammad R. Farahani[3] and Wei Gao[4]

Milan Randič proposed the well-known Randič connectivity index, defined on the ground of vertex degrees $R(G) = \sum_{e=uv\in E(G)} (d_u d_v)^{\frac{-1}{2}}$*. In 2008, B. Zhou and N. Trinajstic proposed another connectivity index, named the Sum-connectivity index* $\chi(G) = \sum_{e=uv\in E(G)} (d_u + d_v)^{\frac{-1}{2}}$*. Substitution of* $\frac{-1}{2}$ *by any real number* α*is called the generalization of these topological indices. In this paper, we obtained some results for general Randič and Sum-connectivity and modify Randič indices for Carbon Nanocones* $CNC_k[n]$*.*

Keywords: Molecular graphs, Randič index, Sum-connectivity index, Modify Randič Index, Carbon Nanocones $CNC_k[n]$

2000 Mathematics Subject Clasification: 05C 12, 05C 90.

1. Introductions

Let G be a molecular graph without directions, multiple edges and loops, the vertex and edge-sets of which are represented by $V(G)$ and $E(G)$, respectively. The distance between any two vertices $u, v \in V(G)$, of the graph G is the length of the shortest path connecting them. It is denoted as $d(u, v)$. The degree of a vertex, $u \in V(G)$, is the number of adjacent vertices to u and we denoted it as d_u. The maximum and minimum degree in a graph G is denoted as Δ and δ, respectively. Any vertex u of a graph G satisfies the following relation

$$0 \leq \delta \leq d_u \leq \Delta \leq n - 1.$$

[1]School of Mathematics and Physics, Anhui Jianzhu University, Hefei 230601, China, e-mail: `liujiabaoad@163.com; liujiabao@ahjzu.edu.cn`

[2]Department of Mathematics, Riphah Institute of Computing and Applied Sciences (RICAS), Riphah International University, Lahore, Pakistan, e-mail: `m.kamran.sms@gmail.com`

[3]Department of Mathematics, Iran University of Science and Technology (IUST), Narmak, Tehran 16844,Iran, e-mail: `MrFarahani88@Gmail.com`

[4]School of Information and Technology, Yunnan Normal University, Kunming, 650500, China, e-mail: `gaowei@ynnu.edu.cn`

So, any edge $uv = e \in E(G)$ satisfies the following inequalities

$$2\delta \le d_u + d_v \le 2\Delta$$
$$\delta^2 \le d_u \times d_v \le 2\Delta^2$$

In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [1-8]. Among topological descriptors connectivity indices are very important and they have a prominent role in chemistry.

Numbers reflecting certain structural features of organic molecules that are obtained from the molecular graph are usually called graph invariants or more commonly topological indices. In other words, an arbitrary topological index is fixed by any automorphism of the graph. There are several topological indices have been defined.

One of the oldest graph invariants are the Wiener index, which was formally introduced by *Harold Wiener* [1] (in 1947). The Wiener index is defined as the sum of distances between any two atoms in the molecules, in terms of bonds and denoted by *W(G).*

$$W(G) = \tfrac{1}{2}\sum_{v\in V(G)}\sum_{u\in V(G)} d(v,u)$$

where $d(u,v)$ denote the distance between vertices u and v in G .

Among the numerous topological indices considered in chemical graph theory, only a few have been found noteworthy in practical application, connectivity index is one of them.

In 1975,*Milan Randiȁ* proposed a structural descriptor called the branching index [9] that later became the well-known Randiȁ connectivity index $R(G)$. Motivated by the definition of Randiȁ connectivity index based on the end-vertex degrees of edges in a graph and is equal to

$$R(G) = \sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

This index has been successfully correlated with physo-chemical properties of organic molecules. Indeed if G is the molecular graph of a saturated hydrocarbon then there is a strong correlation between $R(G)$ and the boiling point of the substance [10]–[14].

Another connectivity indices is the *Sum-Connectivity Index* that introduced by *B. Zhou* and *N. Trinajstič* in 2008 [15, 16]. The sum-connectivity index $\chi(G)$ is defined as the sum over all edges of the graph of the terms $(d_u + d_v)^{-1/2}$ and is equal to

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$$

Recently in 2011, *Z. Dvorak et. al.* proposed a modification of the Randič Index of G and is defined as $R'(G) = \sum_{uv \in E(G)} \frac{1}{\max\{d_u, d_v\}}$ that is more tractable from computational point of view. It is much easier to follow during graph modifications than Randič index see [17] for more details. Some basic properties of these indices can be found in the recent letters. For more study, see reference [18, 19, 20].
The *general Randič index* was introduced by *Kier* et. al. [3] in 1976, which is defined as the sum of the weights $(d_u d_v)^\alpha$ $(\forall \alpha \in \mathbb{R})$ and is equal to $R^\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$

The general sum-connectivity index was introduced by *Zhou* et. al. [16], is equal to $(\forall \alpha \in \mathbb{R})$:

$$\chi^\alpha(G) = \sum_{e=uv \in E(G)} (d_u + d_v)^\alpha$$

Then $\chi_{-1/2}(G)$ is the sum-connectivity index.

For a simple graph G the first and second Zagreb indices of a graph G are defined as: [2]
$M_1(G) = \sum_{v \in E(G)} (d_u)^2 = \sum_{e=uv \in E(G)} (d_u + d_v)$

$M_2(G) = \sum_{e=uv \in E(G)} (d_u \times d_v)$.

The first general Zagreb index of G is introduced by Li and Gutman [21] and is defined as:

$$M_1^\alpha(G) = \sum_{v \in E(G)} (d_v)^\alpha = \sum_{e=uv \in E(G)} \left(d_u^{(\alpha-1)} + d_v^{(\alpha-1)}\right)$$

Where α is a real number with $\alpha \neq 0$ and $\alpha \neq 1$.
Since 1968, carbons Nanocones have been determined on the skin of naturally

arising graphite [22]. Carbon nanostructures earned extraordinary attention due to their possible use in many utilization including, nano-electronic devices, biosensors, and chemical probes [23, 24]. We refer [25]–[41] for some results on carbon Nanocones.

In this paper, we investigate the connectivity topological indices, and computed some formulas for the *Randiċ, sum-connectivity, modify Randiċ*, general *Randiċ and cum-connectivity,* indices of carbon nanocones $CNC_k[n]$.

2. **Results and Discussion**

For a simple molecular graph G, we partition the edge set $E(G)$ based on the degrees of end vertices of each edge as follows

$$\forall j : 2\delta \leq j \leq 2\Delta,\ E_j = \{uv \in E\,(G)\,|d_u + d_v\}$$
$$\forall k : \delta^2 \leq k \leq 2\Delta^2,\ E^*_k = \{uv = e \in E\,(G)\,|d_u \times d_v = k\}$$

$|E_j|, |E^*_k|$ represent the number of elements in the sets E_j and E^*_k.

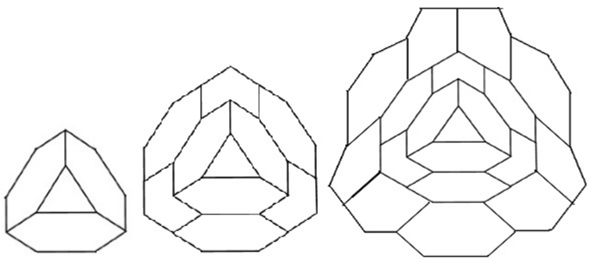

FIGURE 1. Molecular graphs of $CNC_3[1]$, $CNC_3[2]$ and $CNC_3[3]$.

Theorem 2.1. *Let $CNC_3[n]$ be a graph, here n is any positive integer. Then*

$$R^\alpha\,(CNC_3[n]) = 3 \cdot 4^\alpha + (n-1) \cdot 6^{\alpha+1} + \left(3n^2 - 5n + 2\right)\left(\frac{3^{2\alpha+1}}{2}\right),$$

$$\chi_\alpha\,(CNC_3[n]) = 3 \cdot 4^\alpha + 6\,(n-1) \cdot 5^\alpha + \left(9n^2 - 15n + 6\right)\left(\frac{6^\alpha}{2}\right),$$

$$R^{'}\,(CNC_3[n]) = \frac{3n^2 - n + 1}{2}.$$

where α is any real non-zero number.

Proof. For positive integer n, suppose $CNC_3[n]$ is the n^{th} representative of carbon nanocones Fig. 1. The n^{th} representative of nanocones contain $3n^2$ vertices and $\frac{n}{2}\,(9n-3)$ edges. The graph of $CNC_3[n]$ contain the vertices with degree 2 or 3. The partition of edge set based on the end vertices of edges is as

$$E_4 = \{uv \in E(CNC_3[n]) | d_u + d_v = 4\}$$
$$E_5 = \{uv \in E(CNC_3[n]) | d_u + d_v = 5\}$$
$$E_6 = \{uv \in E(CNC_3[n]) | d_u + d_v = 6\}$$
$$E_4^* = \{uv \in E(G) | d_u \times d_v = 4\}$$
$$E_6^* = \{uv \in E(G) | d_u \times d_v = 6\}$$
$$E_9^* = \{uv \in E(G) | d_u \times d_v = 9\}$$

and

$$|E_4| = |E_4^*| = 3$$
$$|E_5| = |E_6^*| = 6(n-1)$$
$$|E_6| = |E_9^*| = \tfrac{9}{2}n^2 - \tfrac{15}{2}n + 3.$$

from the above information we have the following

$$\begin{aligned}
&R^\alpha(CNC_3[n]) = \textstyle\sum_{uv\in E(CNC_3[n])} (d_u \times d_v)^\alpha \\
&= \textstyle\sum_{uv\in E_4^*} (d_u \times d_v)^\alpha + \sum_{uv\in E_6^*} (d_u \times d_v)^\alpha + \sum_{uv\in E_9^*} (d_u \times d_v)^\alpha \\
&= \textstyle\sum_{j=4,6,9} j^\alpha \times |E_j^*| \\
&= 4^\alpha |E_4^*| + 6^\alpha |E_6^*| + 9^\alpha |E_9^*| \\
&= 4^\alpha \times 3 + 6^\alpha \times 6(n-1) + 9^\alpha \times \left(\tfrac{9n^2-15n+6}{2}\right) \\
&= 3 \cdot 4^\alpha + (n-1) \cdot 6^{\alpha+1} + (3n^2 - 5n + 2)\left(\tfrac{3^{2\alpha+1}}{2}\right)
\end{aligned}$$

$$\begin{aligned}
&\chi^\alpha(CNC_3[n]) = \textstyle\sum_{uv\in E(CNC_3[n])} (d_u + d_v)^\alpha \\
&= \textstyle\sum_{uv\in E_4} (d_u + d_v)^\alpha + \sum_{uv\in E_5} (d_u + d_v)^\alpha + \sum_{uv\in E_6} (d_u + d_v)^\alpha \\
&= \textstyle\sum_{j=4,5,6} j^\alpha \times |E_j| \\
&= 4^\alpha |E_4| + 5^\alpha |E_5| + 6^\alpha |E_6| \\
&= 4^\alpha \times 3 + 5^\alpha \times 6(n-1) + 6^\alpha \times \left(\tfrac{9n^2-15n+6}{2}\right) \\
&= 3 \cdot 4^\alpha + 6(n-1) \cdot 5^\alpha + (9n^2 - 15n + 6)\left(\tfrac{6^\alpha}{2}\right)
\end{aligned}$$

$$\begin{aligned}
&R'(CNC_3[n]) = \textstyle\sum_{uv\in E(CNC_3[n])} \frac{1}{\max\{d_u,d_v\}} \\
&= \textstyle\sum_{uv\in E_4} \frac{1}{\max\{d_u,d_v\}} + \sum_{uv\in E_5\ or\ uv\in E_6} \frac{1}{\max\{d_u,d_v\}} \\
&= \tfrac{3}{2} + \tfrac{9n^2-3n-6}{6} \\
&= \tfrac{3n^2-n+1}{2}.
\end{aligned}$$

Hence, the proof is complete. □

Theorem 2.2. *Let $CNC_4[n]$ be a graph, where n is any positive integer. Then* $\forall \alpha \in \mathbb{R}$

$$R^\alpha(CNC_4[n]) = 4^{\alpha+1} + 8(n-1) \cdot 6^\alpha + \left(6n^2 - 10n + 4\right) \cdot 9^\alpha,$$
$$\chi_\alpha(CNC_4[n]) = 4^{\alpha+1} + 8(n-1) \cdot 5^\alpha + \left(6n^2 - 10n + 4\right) 6^\alpha,$$

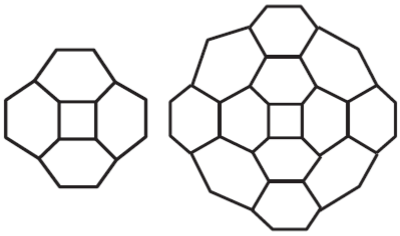

FIGURE 2. The molecular graph of $CNC_4[1]$ and $CNC_4[2]$.

$$R^{'}(CNC_4[n]) = \frac{6n^2-2n+2}{3}.$$

Proof. For positive integer n, suppose $CNC_4[n]$ is the n^{th} representative of carbon nanocones Fig. 2. The n^{th} representative of this Nanonoces contains $4n^2$ vertices and $2n(3n-1)$ edges. The graph of $CNC_4[n]$ contain the vertices with degree 2 or 3. The partition of edge set based on the end vertices degree of an edge is as follows

$$|E_4| = |E_4^*| = 4$$
$$|E_5| = |E_6^*| = 8(n-1)$$
$$|E_6| = |E_9^*| = 6n^2-10n+4$$

From the above information we have

$$R^{\alpha}(CNC_4[n]) = \sum_{uv\in E(CNC_4[n])}(d_u\times d_v)^{\alpha}$$
$$= \sum_{uv\in E_4^*}(d_u\times d_v)^{\alpha} + \sum_{uv\in E_6^*}(d_u\times d_v)^{\alpha} + \sum_{uv\in E_9^*}(d_u\times d_v)^{\alpha}$$
$$= \sum_{j=4,6,9} j^{\alpha}\times|E_j^*|$$
$$= 4^{\alpha}|E_4^*| + 6^{\alpha}|E_6^*| + 9^{\alpha}|E_9^*|$$
$$= 4^{\alpha}\times 4 + 6^{\alpha}\times 8(n-1) + 9^{\alpha}\times(6n^2-10n+4)$$
$$= 4^{\alpha+1} + 8(n-1)\cdot 6^{\alpha} + (6n^2-10n+4)\cdot 9^{\alpha}$$

$$\chi^{\alpha}(CNC_4[n]) = \sum_{uv\in E(CNC_4[n])}(d_u+d_v)^{\alpha}$$
$$= \sum_{uv\in E_4}(d_u+d_v)^{\alpha} + \sum_{uv\in E_5}(d_u+d_v)^{\alpha} + \sum_{uv\in E_6}(d_u+d_v)^{\alpha}$$
$$= \sum_{j=4,5,6} j^{\alpha}\times|E_j|$$
$$= 4^{\alpha}|E_4| + 5^{\alpha}|E_5| + 6^{\alpha}|E_6|$$
$$= 4^{\alpha}\times 4 + 5^{\alpha}\times 8(n-1) + 6^{\alpha}\times(6n^2-10n+4)$$
$$= 4^{\alpha+1} + 8(n-1)\cdot 5^{\alpha} + (6n^2-10n+4)\,6^{\alpha}$$

$$R^{'}(CNC_4[n]) = \sum_{uv\in E(CNC_4[n])}\frac{1}{\max\{d_u,d_v\}}$$
$$= \sum_{uv\in E_4}\frac{1}{\max\{d_u,d_v\}} + \sum_{uv\in E_5\, or\, uv\in E_6}\frac{1}{\max\{d_u,d_v\}}$$
$$= \frac{4}{2} + \frac{6n^2-2n-4}{3}$$
$$= \frac{6n^2-2n+2}{3}.$$

Hence, the proof is complete. □

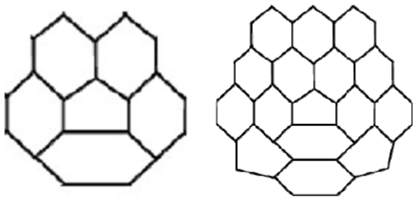

FIGURE 3. First three members of First two members of First two members of $CNC_5[n]$.

Theorem 2.3. *Let $CNC_5[n]$ be a graph, where n is any positive integer. Then*

$$R^\alpha\left(CNC_5[n]\right) = 5\cdot 4^\alpha + 10\,(n-1)\cdot 6^\alpha + \left(\frac{15n^2-25n+10}{2}\right)\cdot 9^\alpha,$$

$$\chi_\alpha\left(CNC_5[n]\right) = 5\cdot 4^\alpha + 10\,(n-1)\cdot 5^\alpha + \left(\frac{15n^2-25n+10}{2}\right)6^\alpha,$$

$$R^{'}\left(CNC_5[n]\right) = \frac{15n^2-5n+23}{6}.$$

where α is any real number.

Proof. For positive integer n, suppose $CNC_5[n]$ is the n^{th} representative of carbon nanocones Fig. 3. This class of Nanonoces contain $5n^2$ vertices and $\frac{15n^2-5n}{2}$ edges. The graph of $CNC_5[n]$ contain the vertices with degree 2 or 3. As in the previous, we partitioned the edge set of $E\left(CNC_5\left[n\right]\right)$ have the following cardinalities as follows

$$\begin{array}{l} |E_4| = |E_4^*| = 5 \\ |E_5| = |E_6^*| = 10\,(n-1) \\ |E_6| = |E_9^*| = \frac{15n^2-25n+10}{2} \end{array}$$

$$\begin{array}{l} R^\alpha\left(CNC_5\left[n\right]\right) = \sum_{uv\in E(CNC_5[n])}\left(d_u\times d_v\right)^\alpha \\ = \sum_{uv\in E_4^*}\left(d_u\times d_v\right)^\alpha + \sum_{uv\in E_6^*}\left(d_u\times d_v\right)^\alpha + \sum_{uv\in E_9^*}\left(d_u\times d_v\right)^\alpha \\ = \sum_{j=4,6,9} j^\alpha \times |E_j^*| \\ = 4^\alpha|E_4^*| + 6^\alpha|E_6^*| + 9^\alpha|E_9^*| \\ = 4^\alpha\times 5 + 6^\alpha\times 10\,(n-1) + 9^\alpha\times\left(\frac{15n^2-25n+10}{2}\right) \\ = 5\cdot 4^\alpha + 10\,(n-1)\cdot 6^\alpha + \left(\frac{15n^2-25n+10}{2}\right)\cdot 9^\alpha \end{array}$$

$$\chi^{\alpha}(CNC_5[n]) = \sum_{uv\in E(CNC_5[n])}(d_u+d_v)^{\alpha}$$
$$= \sum_{uv\in E_4}(d_u+d_v)^{\alpha} + \sum_{uv\in E_5}(d_u+d_v)^{\alpha} + \sum_{uv\in E_6}(d_u+d_v)^{\alpha}$$
$$= \sum_{j=4,5,6} j^{\alpha} \times |E_j|$$
$$= 4^{\alpha}|E_4| + 5^{\alpha}|E_5| + 6^{\alpha}|E_6|$$
$$= 4^{\alpha}\times 5 + 5^{\alpha}\times 10(n-1) + 6^{\alpha}\times\left(\frac{15n^2-25n+10}{2}\right)$$
$$= 5\cdot 4^{\alpha} + 10(n-1)\cdot 5^{\alpha} + \left(\frac{15n^2-25n+10}{2}\right)6^{\alpha}$$

$$R'(CNC_5[n]) = \sum_{uv\in E(CNC_5[n])}\frac{1}{\max\{d_u,d_v\}}$$
$$= \sum_{uv\in E_4}\frac{1}{\max\{d_u,d_v\}} + \sum_{uv\in E_5\, or\, uv\in E_6}\frac{1}{\max\{d_u,d_v\}}$$
$$= \frac{5}{2} + \frac{15n^2-5n+8}{6}$$
$$= \frac{15n^2-5n+23}{6}$$

□

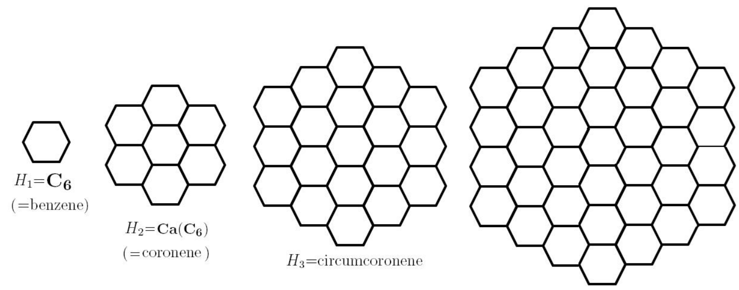

FIGURE 4. First three members of $CNC_6[n]$.

Theorem 2.4. *Let $CNC_6[n]$ be a graph, where n is any positive integer. Then*

$$R^{\alpha}(CNC_6[n]) = 6\cdot 4^{\alpha} + 12(n-1)\cdot 6^{\alpha} + \left(9n^2-15n+6\right)\cdot 9^{\alpha},$$
$$\chi_{\alpha}(CNC_6[n]) = 6\cdot 4^{\alpha} + 12(n-1)\cdot 5^{\alpha} + \left(9n^2-15n+6\right)6^{\alpha},$$
$$R'(CNC_6[n]) = 3n^2-5n+5.$$

where α is any real number.

Proof. Let $CNC_6[n]$ be the n^{th} member of Carbon Nanocones, where n is any positive integer. This class of Nanonoces contain $6n^2$ vertices and $9n^2-3n$ edges. The graph of $CNC_6[n]$ contain the vertices with degree 2 or 3. Based on the degree of the vertices, the partitions of the edge set $E(CNC_6[n])$ have the following cardinalities as follows

$$|E_4| = |E_4^*| = 6$$
$$|E_5| = |E_6^*| = 12(n-1)$$
$$|E_6| = |E_9^*| = 9n^2-15n+6$$

With the help of this partition we can obtain our desired results

$$R^{\alpha}\left(CNC_6\left[n\right]\right)=\sum_{uv\in E(CNC_6[n])}\left(d_u\times d_v\right)^{\alpha}$$
$$=\sum_{uv\in E_4^*}\left(d_u\times d_v\right)^{\alpha}+\sum_{uv\in E_6^*}\left(d_u\times d_v\right)^{\alpha}+\sum_{uv\in E_9^*}\left(d_u\times d_v\right)^{\alpha}$$
$$=\sum_{j=4,6,9}j^{\alpha}\times|E_j^*|$$
$$=4^{\alpha}|E_4^*|+6^{\alpha}|E_6^*|+9^{\alpha}|E_9^*|$$
$$=4^{\alpha}\times 6+6^{\alpha}\times 12\left(n-1\right)+9^{\alpha}\times\left(9n^2-15n+6\right)$$
$$=6\cdot 4^{\alpha}+12\left(n-1\right)\cdot 6^{\alpha}+\left(9n^2-15n+6\right)\cdot 9^{\alpha}$$

$$\chi^{\alpha}\left(CNC_6\left[n\right]\right)=\sum_{uv\in E(CNC_6[n])}\left(d_u+d_v\right)^{\alpha}$$
$$=\sum_{uv\in E_4}\left(d_u+d_v\right)^{\alpha}+\sum_{uv\in E_5}\left(d_u+d_v\right)^{\alpha}+\sum_{uv\in E_6}\left(d_u+d_v\right)^{\alpha}$$
$$=\sum_{j=4,5,6}j^{\alpha}\times|E_j|$$
$$=4^{\alpha}|E_4|+5^{\alpha}|E_5|+6^{\alpha}|E_6|$$
$$=4^{\alpha}\times 6+5^{\alpha}\times 12\left(n-1\right)+6^{\alpha}\times\left(9n^2-15n+6\right)$$
$$=6\cdot 4^{\alpha}+12\left(n-1\right)\cdot 5^{\alpha}+\left(9n^2-15n+6\right)6^{\alpha}$$

$$R'\left(CNC_6\left[n\right]\right)=\sum_{uv\in E(CNC_6[n])}\frac{1}{\max\{d_u,d_v\}}$$
$$=\sum_{uv\in E_4}\frac{1}{\max\{d_u,d_v\}}+\sum_{uv\in E_5\ or\ uv\in E_6}\frac{1}{\max\{d_u,d_v\}}$$
$$=\frac{6}{2}+\frac{9n^2-15n+6}{3}$$
$$=3n^2-5n+5.$$

Hence, the proof is complete. □

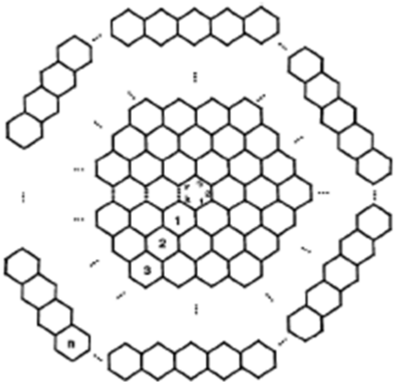

FIGURE 5. A general representation of Carbon Nanocones $CNC_k[n]$ $\forall k,n\in N\&k=3$.

Theorem 2.5. *Let $\alpha\in R,n\in N$ and $k=3$, and $CNC_4[n]$ be a graph. Then :*

$$R^{\alpha}\left(CNC_k[n]\right)=4^{\alpha}k+2k\left(n-1\right)6^{\alpha}+\frac{9^{\alpha}}{2}k\left(3n^2-5n+2\right),$$
$$\chi_{\alpha}\left(CNC_k[n]\right)=4^{\alpha}k+2\left(n-1\right)5^{\alpha}+\frac{6^{\alpha}}{2}\left(3n^2-5n+2\right)k,$$

$$R^{'}\left(CNC_k[n]\right) = \left(\frac{n^2}{2} + \frac{n}{3} - \frac{1}{3}\right) k.$$

Proof. Let the molecular graph of Carbon Nanocones $CNC_k[n]$ Fig. 6, with kn^2 vertices and $\frac{k}{2}n\left(3n-1\right)$ edges. The graph of $CNC_k[n]$ contain the vertices with degree 2 or 3. Based on the degree of the vertices, we have three edge partitions of $E\left(CNC_k\left[n\right]\right)$ as follows

$|E_4|$=$|E_4{}^*|$=k,

$|E_5|$=$|E_6{}^*|$=$2k(n\text{-}1)$,

$|E_6|$=$|E_9{}^*|$=$\frac{3}{2}kn^2$-$\frac{5}{2}kn$+k=$\frac{1}{2}k(3n^2\text{-}5n\text{+}2)$.

Here by these partitions, we can obtain our desired results $\forall\alpha \in \mathbb{R}$, $\forall k, n \in N \& k = 3$.

$$\begin{aligned}
&R^{\alpha}\left(CNC_k\left[n\right]\right) = \textstyle\sum_{uv\in E(CNC_k[n])}\left(d_u \times d_v\right)^{\alpha}\\
&= \textstyle\sum_{uv\in E_4^*}\left(d_u \times d_v\right)^{\alpha} + \sum_{uv\in E_6^*}\left(d_u \times d_v\right)^{\alpha} + \sum_{uv\in E_9^*}\left(d_u \times d_v\right)^{\alpha}\\
&= \textstyle\sum_{j=4,6,9} j^{\alpha} \times |E_j^*|\\
&= 4^{\alpha}|E_4^*| + 6^{\alpha}|E_6^*| + 9^{\alpha}|E_9^*|\\
&= 4^{\alpha} \times k + 6^{\alpha} \times 2k\left(n-1\right) + 9^{\alpha}\left(k\left(3n^2-5n+2\right)\right)\\
&= 4^{\alpha}k + 2k\left(n-1\right)6^{\alpha} + \tfrac{9^{\alpha}}{2}k\left(3n^2-5n+2\right)
\end{aligned}$$

$$\begin{aligned}
&\chi^{\alpha}\left(CNC_k\left[n\right]\right) = \textstyle\sum_{uv\in E(CNC_k[n])}\left(d_u + d_v\right)^{\alpha}\\
&= \textstyle\sum_{uv\in E_4}\left(d_u + d_v\right)^{\alpha} + \sum_{uv\in E_5}\left(d_u + d_v\right)^{\alpha} + \sum_{uv\in E_6}\left(d_u + d_v\right)^{\alpha}\\
&= \textstyle\sum_{j=4,5,6} j^{\alpha} \times |E_j|\\
&= 4^{\alpha}|E_4| + 5^{\alpha}|E_5| + 6^{\alpha}|E_6|\\
&= 4^{\alpha} \times k + 5^{\alpha} \times 2k\left(n-1\right) + 6^{\alpha} \times \left(k\left(3n^2-5n+2\right)\right)\\
&= 4^{\alpha}k + 2k\left(n-1\right)5^{\alpha} + \tfrac{6^{\alpha}}{2}k\left(3n^2-5n+2\right)
\end{aligned}$$

$$\begin{aligned}
&R^{'}\left(CNC_k\left[n\right]\right) = \textstyle\sum_{uv\in E(CNC_k[n])}\frac{1}{\max\{d_u,d_v\}}\\
&= \textstyle\sum_{uv\in E_4}\frac{1}{\max\{d_u,d_v\}} + \sum_{uv\in E_5\, or\, uv\in E_6}\frac{1}{\max\{d_u,d_v\}}\\
&= \tfrac{|E_4|}{2} + \tfrac{|E_5|+|E_6|}{3}\\
&= \tfrac{k}{2} + \tfrac{2k(n-1)+k\left(3n^2-5n+2\right)}{3}\\
&= \left(\tfrac{n^2}{2} + \tfrac{n}{3} - \tfrac{1}{3}\right)k.
\end{aligned}$$

□

From the above results we have the following corollaries.

Corollary 2.1. *The Randiċ index of to*

$$
\begin{aligned}
R\left(CNC_3\left[n\right]\right) &= \tfrac{3}{2}n^2 + \left(\sqrt{6}-\tfrac{5}{2}\right)n + \left(\sqrt{6}+\tfrac{5}{2}\right)\\
R\left(CNC_4\left[n\right]\right) &= 2n^2 + \left(\tfrac{8}{\sqrt{6}}-\tfrac{10}{3}\right)n + \left(\tfrac{10}{3}-\tfrac{8}{\sqrt{6}}\right)\\
R\left(CNC_5\left[n\right]\right) &= \tfrac{5}{2}n^2 + \left(\tfrac{10}{\sqrt{6}}-\tfrac{25}{2}\right)n + \left(\tfrac{25}{6}-\tfrac{10}{\sqrt{6}}\right)\\
R\left(CNC_6\left[n\right]\right) &= 3n^2 + \left(2\sqrt{6}-5\right)n + \left(5-2\sqrt{6}\right)\\
&\vdots\\
R\left(CNC_k[n]\right) &= \left(\tfrac{9}{2}n^2 + (2\sqrt{6}-\tfrac{15}{2})n + \left(7-2\sqrt{6}\right)\right)k
\end{aligned}
$$

Corollary 2.2. *The sum-connectivity index of is equal to*

$$
\begin{aligned}
\chi\left(CNC_3\left[n\right]\right) &= \tfrac{9}{2\sqrt{6}}n^2 + \left(6\sqrt{5}-\tfrac{15}{2\sqrt{6}}\right)n + \left(\tfrac{3+\sqrt{6}}{2}\right)\\
\chi\left(CNC_4\left[n\right]\right) &= \sqrt{6}n^2 + \left(\tfrac{8\sqrt{5}}{5}-\tfrac{5\sqrt{6}}{3}\right)n + \left(2+\tfrac{2\sqrt{6}}{3}-\tfrac{8\sqrt{5}}{5}\right)\\
\chi\left(CNC_5\left[n\right]\right) &= \tfrac{15\sqrt{6}}{12}n^2 + \left(2\sqrt{5}-\tfrac{25\sqrt{6}}{12}\right)n + \left(\tfrac{5}{4}-2\sqrt{5}+\tfrac{5\sqrt{6}}{6}\right)\\
\chi\left(CNC_6\left[n\right]\right) &= \tfrac{3\sqrt{6}}{2}n^2 + \left(\tfrac{12\sqrt{5}}{5}-\tfrac{5\sqrt{6}}{2}\right)n + \left(3+\sqrt{6}-\tfrac{12\sqrt{5}}{5}\right)\\
&\vdots\\
\chi\left(CNC_k[n]\right) &= 2k + 2\left(n-1\right)\sqrt{5} + \tfrac{\sqrt{6}}{2}\left(3n^2-5n+2\right)k\\
&= \left(\tfrac{3\sqrt{6}}{2}n^2 + \left(2\sqrt{5}-\tfrac{5\sqrt{6}}{2}\right)n + \left(2+\sqrt{6}-2\sqrt{5}\right)\right)k
\end{aligned}
$$

Corollary 2.3. *The first Zagreb index of equal to*

$$
\begin{aligned}
M_1\left(CNC_3\left[n\right]\right) &= 27n^2 - 15n\\
M_1\left(CNC_4\left[n\right]\right) &= 36n^2 - 20n + 48\\
M_1\left(CNC_5\left[n\right]\right) &= 45n^2 - 25n\\
M_1\left(CNC_6\left[n\right]\right) &= 54n^2 - 30n + 72\\
&\vdots\\
M_1\left(CNC_k\left[n\right]\right) &= 9kn^2 - 5kn.
\end{aligned}
$$

Corollary 2.4. *The second Zagreb index of equal to*

$$
\begin{aligned}
M_2\left(CNC_3\left[n\right]\right) &= \tfrac{81}{2}n^2 - \tfrac{63}{2}n + 3\\
M_2\left(CNC_4\left[n\right]\right) &= 54n^2 + 43n + 4\\
M_2\left(CNC_5\left[n\right]\right) &= \tfrac{135}{2}n^2 - \tfrac{105}{2}n + 5\\
M_2\left(CNC_6\left[n\right]\right) &= 81n^2 - 63n + 6\\
&\vdots\\
M_2\left(CNC_k\left[n\right]\right) &= k\left(n^2-n+1\right). \blacksquare
\end{aligned}
$$

3. Conclusions

Topological indices have found application in different regions of science, material science, arithmetic, informatics, biology, however their most critical use to date is in the non-exact Quantitative Structure-Property Relationships

(QSPR) and Quantitative Structure-Activity Relationships (QSAR). Our results can help to guess properties of Carbon Nanocones, for example: The Randiĉ index is a standout amongst the frequently connected sub-atomic structure descriptor. The Randiĉ index demonstrates great relationship with every single physical property of alkanes, aside from their liquefying focuses with correlation coefficient value r=0:219. Further, the value of r lies between 0.881 to 0.995. Randiĉ index has high connection with heat of vaporization of the alkanes with r=0:995. The foreseeing intensity of GA for the physical properties of alkanes is similarly great as Randiĉ index. The value of r lies between 0.889 to 0.987 aside from melting point of alkanes, with r=0.235. Shockingly, we could see that the connection of GA with heat of vaporization of alkanes is extremely high with r=0.9871.

References

[1] *H. Wiener*, Structural determination of paraffin boiling points, J. Am. Chem. Soc., **69**, (1947), 17-20.

[2] *I. Gutman, N. Trinajstiĉ,* Graph theory and molecular orbitals. III. Total π-electron energy of alternant hydrocarbons. Chem. Phys. Lett., **17**, (1972), 535–538.

[3] *L.B. Kier, L.H. Hall,* Molecular Connectivity in Chemistry and Drug Research. Academic Press, New York, (1976).

[4] *L.B. Kier, L.H. Hall,* Molecular Connectivity in Structure-Activity Analysis. Research Studies Press/Wiley, Letchworth/New York, (1986).

[5] *N. Trinajstiĉ,* Chemical Graph Theory. (2nd edition). CRC Press, Boca Raton, FL. (1992).

[6] *N. Trinajstiĉ, I. Gutman,* Mathematical Chemistry, Croat. Chem. Acta, **75** (2002), 329-356.

[7] *R. Todeschini and V. Consonni,* Handbook of Molecular Descriptors, Weinheim, Wiley-VCH, (2000).

[8] *D. B. West*, Introduction to Graph theory, Prentice Hall, Upper Saddle River, (1996).

[9] *M. Randiĉ*, On the characterization of molecular branching. J. Am. Chem. Soc., **97** (1975), No. 23, 6609-6615.

[10] *Z. Mihali, N. Trinajstiĉ,* A graph-theoretical approach to structure-property relationships. J. Chem. Educ., **699**, (1992), No. 9, 701.

[11] *D. Morales, O. Araujo.* On the search for the best correlation between graph theoretical invariants and physicochemical properties. J. Math. Chem., **13**, (1993), 95.

[12] *M. Randic, P.J. Hansen, P.C. Jurs*, Search for useful graph theoretical invariants of molecular structure. J. Chem. Inf. Comput. Sci., **28**, (1988), 60-68.

[13] *E. Estrada*, Connectivity polynomial and long-range contributions in the molecular connectivity model. Chem. Phys. Lett., **312**, (1999), 556-560.

[14] *E. Estrada*, Graph theoretical invariant of Randic revisited. J. Chem. Inf. Comput. Sci., **35**, (1995), 1022-1025.

[15] *B. Zhou and N. Trinajstiĉ*, On a novel connectivity index. J. Math. Chem., **46**, (2009), 1252-1270.

[16] *B. Zhou and N. Trinajstiĉ*, On general sum-connectivity index. J. Math. Chem., **47**, (2010), 210-218.

[17] *Z. Dvorak, B. Lidicky and R. Skrekovski*, Randic index and the diameter of a graph, European J. Combin., **32**, (2011), 434-442.

[18] *F. Ma and H. Deng*, On the sum-connectivity index of cacti, Math. Com. Mod., **24** (2011), No. 1-2, 497-507.

[19] *M.R. Farahani*, Some Connectivity Indices and Zagreb Index of Polyhex Nanotubes. Acta Chim. Slov., **59**, (2012), 779–783.

[20] *M.R. Farahani*, Computing some connectivity indices of Nanotubes. Adv. Mater. Corrosion., **1**, (2012), 57-60.

[21] *X. Li, I. Gutman*, Mathematical aspects of Randic type molecular structure descriptors, Univ. Kragujevac, Kragujevac, (2006).

[22] *J. Gillot, W. Bollmann, B. Lux*, Cristaux de graphite en forme de cigare et a structure conique. Carbon, **6**, (1968), 381-384.

[23] *S. Iijima*, Helical Microtubules of Graphitic Carbon. Nature, **354**, (1991) 56-58.

[24] *M. Yudasaka, S. Iijima, V. H. Crespi*, Single-Wall Carbon Nanohorns and Nanocones. Topics in Applied Physics, **111**, (2008), 605-629.

[25] *M. Ge and K. Sattler*, Chemical Physics Letters Observation of fullerene cones, Chem. Phy. Let., **220**, (1994), No. (3–5), 192-196.

[26] *A.R. Ashrafi, H. Saati*, PI and Szeged indices of one-pentagonal carbon Nanocones. J. Comput. Theor. Nanosci., **4**, (2007), 1-3.

[27] *M. H. Khalifeh, H. Y. Azari, A. R. Ashrafi*, A method for computing the Wiener index of one-pentagonal carbon Nanocones, Current Nanoscience, **6**, (2010), 155-157.

[28] *A. Nejati, M. Alaeiyan*, The edge version of MEC index of one-pentagonal carbon Nanocones, Bul. Chem. Com., **46**, (2014), No. 3, 462-464.

[29] *M. Ghorbani, M. Jalali*, The Vertex PI, Szeged and Omega Polynomials of Carbon Nanocones $CNC_4[n]$. MATCH Commun. Math. Comput. Chem., **62**, (2009), No. 2, 353-362.

[30] *S. Wang, B. Wei*, Multiplicative Zagreb indices of Cacti, Discrete Math., Algorithms and Appl., **8**, (2016), No. 3, 1650040.

[31] *C. Wang, S. Wang, B. Wei*, Cacti with Extremal PI Index, Transactions on Combinatorics, **5**. (2016), No. 4, 1-8.

[32] *S. Wang, B. Wei*, Multiplicative Zagreb indices of k-trees, Discrete Appl. Math., **180**, (2015), 168-175.

[33] *S. Wang, J.-B. Liu, C. Wang, S. Hayat*, Further results on computation of topological indices of certain networks, IET Control Theory and Applications, **11** (2017), No. 13, 2065-2071.

[34] *S. Wang, M. R. Farahani, M. R. Kanna, M. K. Jamil, R. P. Kumar*, The Wiener Index and the Hosoya Polynomial of the Jahangir Graphs, Applied and Computational Mathematics, **5**, (2016), 138-141.

[35] *W. Gao, M.R. Farahani, M. Imran*, On The Edges Version of ABC and GA indices of Nanocones. J. Comput. Theor. Nanosci., **13**, (2016), No. 10, 6741-6746.

[36] *W. Gao, M.R. Farahani, M.K. Jamil, M.K. Siddiqui*, On the First and Second Zagreb and first and Second Hyper-Zagreb indices of Carbon Nanocones $CNC_k[n]$. J. Comput. Theor. Nanosci., **1313**, (2016), No. 10, 7475-7482.

[37] *L. Yan, M.R. Farahani, W. Gao*, Distance-based Indices Computation of Symmetry Molecular Structures. Open J. Math. Sci., **2**, (2018), No. 1, 323-337.

[38] *M. Imran, A. Asghar, A.Q. Baig*, On Graph Invariants of Oxide Network. Eng. Appl. Sci. Lett., **1**, (2018), No. 1, 23-28.

[39] *W. Gao, A. Asghar, W. Nazeer*, Computing Degree-Based Topological Indices of Jahangir Graph. Eng. Appl. Sci. Lett., **1**, (2018), No. 1, 16-22.

[40] *R. Kanabur, S.K. Hosamani*, Some Numerical Invariants Associated with V-phenylenic Nanotube and Nanotori. Eng. Appl. Sci. Lett., **1**, (2018), No. 1, 1-9.

[41] *N. De*, Computing Reformulated First Zagreb Index of Some Chemical Graphs as an Application of Generalized Hierarchical Product of Graphs. Open J. Math. Sci., **2**, (2018), No. 1, 338-350.