Eccentricity Based Topological Invariants of Tightest non-adjacently Configured Stable Pentagonal Structure of Carbon Nanocones

Mian Muhammad Zobair[1], Mehar Ali Malik[2] and Hani Shaker[3]

[1]National University of Sciences and Technology, Islamabad, Pakistan

[2]Department of Mathematics and Statistics,
Riphah International University Lahore, Pakistan

[3]Department of Mathematics,
COMSATS Institute of Information Technology Defence Road, Lahore, Pakistan

Abstract

Conjugated open ended cones in which the configured pentagons are consistent, lies in the circle of Fries Kekule structure [8]. This non-adjacent tightest configuration of pentagons as shown in the Fig. 1 is consistent with a Fries Kekule structure and thus provides the most stable cone. In the study, various topological indices of the same structure in regard of physico-concoction resources and bioactivity of substance mixtures are studied which further helps to study the behavior of chemical compounds. In this regard, Zagreb indices $M_1^*(G)$ and $M_2^*(G)$ of a molecular graph G are used to evaluate the complexity in chemical systems and biological organisms. In this manuscript, we consider two complex families of stable carbon nanocones and compute their ECI, TEI and eccentricity-based Zagreb indices.

Keywords: Nanocones, eccentric-connectivity index, total-eccentricity index, eccentricity-based Zagreb indices.

Classification: 05C12, 05C10.

1 Introduction and preliminary results

Carbon nanocones are funnel shaped structures made up with dominatingly from carbon with at least one dimension having micrometer or smaller scale. Nanocones are structures which have height and base of same magnitudes, this distinguish them from tipped nanowires which have longer than their diameter. Nanocones lye on the graphite surface having many applications in different fields of chemistry, especially in Electron microscopy, in developing solar cells and plasma torch.

Email addresses: zoobi003@hotmail.com (M. M. Zobair). alies.camp@gmail.com (M.A. Malik). hani.uet@gmail.com (Hani Shaker).

Graph theory has given researchers in the field of chemistry a most beneficial apparatuses in terms of topological indices. Atoms as well as molecular compounds can be represented with ease using a molecular graphs. An atomic graph is a delineation of the basic equation of a synthetic compound as far as graph hypothesis whose vertices deliver a connection between the molecules of a chemical mixture and its edges relate to synthetic bonds.
Chem-informatics is another subject that is a blend of science, arithmetic, and data science. It thinks about QSAR and QSPR property which can be utilized to foresee natural exercises and to get important results of synthetic mixes. In the QSAR/QSPR contemplate, topological invariants are utilized to an-

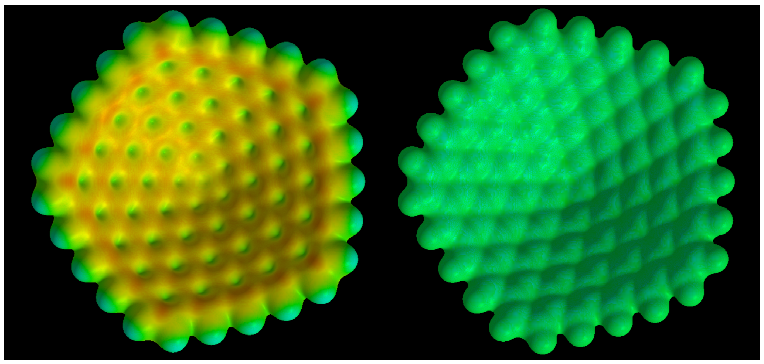

Figure 1: Chemical structures of nanocones originated from a single pentagon, and the structure is viewed from the concave side.

ticipate physico-concoction properties and bioactivity of the substance mixes. A topological invariant is a numeric amount relating to a graph which portrays structure and topology of the diagram exhibiting invariasim if automorphism exists in graph. Among certain real classes of topological invariants such as eccentricity-based, degree-based, counting related polynomials and invariants of graphs, distance-based topological records are of incredible significance and assume an essential part in concoction graphs hypothesis and especially in hypothetical science. Wiener [1] discovered these indices while performing his deliberate efforts on the boiling point of paraffin (a member of the alkaline family) and named it the path number. After that this number was retitled as Wiener index [4] and story of topological indices began.

Let G be a molecular graph of n-vertices having set of vertices $\{v_1, v_2, \ldots, v_n\} \in V(G)$ and an edge set $E(G)$. Length of the shortest (u, v)-path in G is a distance $d(u, v)$ between two vertices $u, v \in V(G)$. For a given vertex $u \in V(G)$, the largest distance between two vertices $u, v \in G$ are defined as eccentricity $\epsilon(u)$. Madan et al. [5, 6] introduced the distance-based topological index of G and named it eccentric-connectivity index (ECI), $\xi(G)$ defined as

$$\xi(G) = \sum_{u \in V(G)} d(u)\epsilon(u). \tag{1.1}$$

When degrees of vertices are not counted, we obtain the total-eccentricity index of the graph G which is defined as

$$\varsigma(G) = \sum_{u \in V(G)} \epsilon(u). \tag{1.2}$$

Ghorbani [10] presented new descriptions of Zagreb indices which were expressed in terms of eccentricity of a molecular graph G given by

$$M_1^*(G) = \sum_{v \in V(G)} (\epsilon(v))^2, \tag{1.3}$$

$$M_2^*(G) = \sum_{uv \in E(G)} \epsilon(u)\epsilon(v). \tag{1.4}$$

Recently, Farahani et al. [9] studied the reverse ECI for a family of nanocones and fullerene structures. Rostami et al [13] found important topological indices for theoretical study of two types of nanostar dendrimers which helps in drug delivery problems. Zobair et al. [2] has studied the eccentricity based topological invariants of triangulane dendrimers and computed eccentricity based ECI, $MECI$, TE and Zagreb indices which are used to predict the bioactivity of chemical compounds. Zobair et al in [3] studied the eccentricity based toplogical invariants of dendrimers and also calculated the Polynomial structure of Benzene ring embedded in periodic-type surface in 2-dimension. Madanshekaf and Ghaneei found the second-order connectivity index of dendrimer nanostars which are important in supra-molecular chemistry, particularly in host guest reactions and self-assembly processes. Khaksar et al in [15] studied the ABC and GA indices of two types of nanocones. Motivation of subject paper comes from the fact that now it is conceivable to make consummate conical carbon nanostructures in a general sense extraordinary from the other nanocarbon structures, remarkably buckyballs and nanotubes [8]. Carbonic cones are acknowledged in distinct five extraordinary structures.

Saheli et al [7] found the eccentricity of a class of nanocone with one pentagon at the centre of cone. In this paper, we discussed the next complicated families of cones based on second and third generation of stable pentagonal cones. THe subject study is a family of five different tightest non-adjacent configuration of the stable pentagons comprising of bended graphite sheets framed as open cones in which one to five carbon pentagons are located at the tip with progressively smaller cone edges, respectively. The nucleation and material science of nanocones has been investigated a little up till now. Furthermore, the motivation of manuscript is from the fact that if the distance increasing between the pentagons then it leads to larger and more localized bond stress at the resulting cusps of cones [8]. More pentagons at the tip of cone gives more stable structures of chemical bonding. In this paper we show the key actualities and results on second and third type of carbon.

In this manuscript, we have formulated and derive closed analytical formulas for the distance-based topological invariants such as eccentric-connectivity index, total-eccentricity index and eccentricity-based Zagreb indices of some families of nanocones discussed in the next section.

2 Some families of nanocones

The first molecular graph of the nanocones studied in this section is represented by $SC_1[n]$, where n denotes stage of the growth. The graph of $SC_1[n]$ for $n = 0$ is the core of $SC_1[n]$. The graph of $SC_1[n]$ with three growth stages $(n = 0, 1, 2)$ is shown in Fig. 2. It is to be noted that $SC_1[n]$ is constructed by $4(n+1)$ hexagon at each layer. We have $|V(SC_1[n])| = 4n^2 + 16n + 14$ and $|E(SC_1[n])| = 6n^2 + 22n + 17$. The molecular graph of second type of nanocones is represented by $SC_2[n]$, where n denotes the growth stage. For $n = 0$, the nanocone $SC_2[0]$ represent the core of $SC_2[n]$. The graph of $SC_2[n]$ with three growth stages $(n = 0, 1, 2)$ is shown in Fig. 4. The graph of $SC_2[n]$ contains $3n^2 + 18n + 21$ vertices and $\frac{3}{2}(3n + 14)(n + 1) + 6$ edges.

Next, we find the eccentricity based topological indices of the nanocones discussed in the previous section.

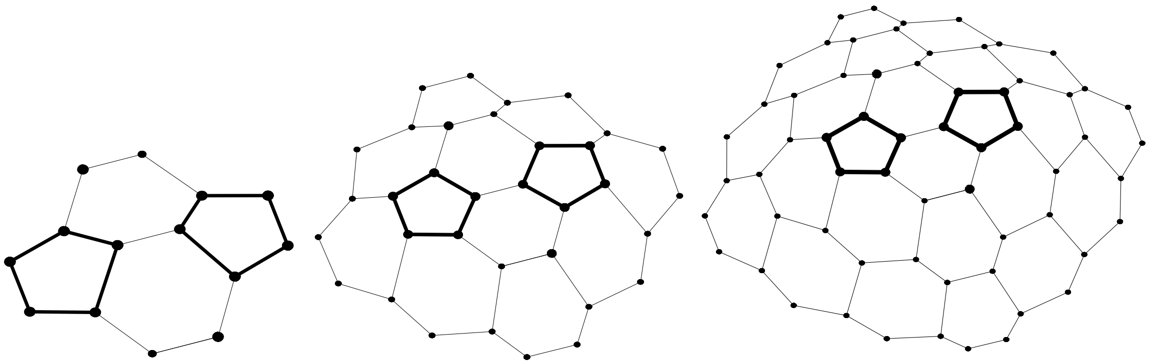

Figure 2: Representation of nanocone $SC_1[n]$ type with two growth stages.

3 Eccentric-connectivity (EC) and total-eccentricity (TE) indices of $SC_1[n]$

In this section, we calculate the ECI and TEI of the first type nanocone $SC_1[n]$, introduced in the previous section. The requisite information required to find the invariants of $SC_1[n]$ are given in Table 1.

$v \in V(G)$	$d(v)$	$\epsilon(v)$	f
w	3	$2n+3$	2
x	3	$2n+5$	4
y	3	$2n+4$	4
z	3	$2n+5$	4
v_1^j $(1 \le j \le n-1)$	3	$2n+2j+5$	8
v_1^j $(j = n)$	2	$2n+2j+5$	8
v_2^j $(1 \le j \le n)$	3	$2n+2j+4$	8
v_i^j $(3 \le i \le j+1,\ 2 \le j \le n-1)$	3	$2n+2j-i+7$	8
v_i^j $(2 \le i \le \frac{n+2}{2}$, $j = n$ and n even$)$	2	$2n+2j-2i+8$	8
v_i^j $(2 \le i \le \frac{n}{2}$, $j = n$ and n even$)$	3	$2n+2j-2i+7$	8
v_i^j $(2 \le i \le \frac{n+3}{2}-1$, $j = n$ and n odd$)$	2	$2n+2j-2i+8$	8
v_i^j $(2 \le i \le \frac{n+3}{2}-1$, $j = n$ and n odd$)$	3	$2n+2j-2i+7$	8
v_{j+2}^j $(1 \le j \le n$ and n even$)$	3	$2n+j+5$	4
v_{j+2}^j $(1 \le j \le n-1$ and n odd$)$	3	$2n+j+5$	4
v_{n+2}^n $(j = n$ and n odd$)$	2	$3n+5$	4

Table 1: Vertices of $SC_1[n]$ with their degrees, eccentricities and frequencies of occurrence, for $1 \le i \le n$.

Theorem 3.1. *The ECI for the core of nanocone $SC_1[n]$ is given by*

$$\xi(SC_1[0]) = 146.$$

Proof. For the nanocone $SC_1[n]$ we use only one quadrant of $SC_1[n]$ by using the concept of symmetry, labeled in Figure 3. One representative from a set of vertices have taken having same size and distance and are labeled by w, x, y, z for $1 \le i \le n$, and their requisite information is given in Table 1.

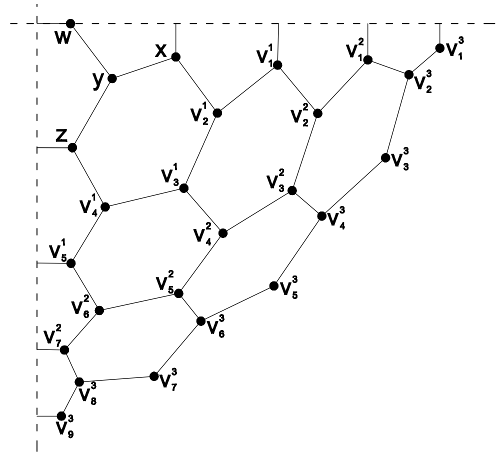

Figure 3: The nanocones $SC_1[n]$ with vertex labeling of a single quadrant.

Using Table 1, ECI of $SC_1[n]$ for $n = 0$ is given by.

$$\begin{aligned}\xi(SC_1[n]) &= \sum_{u \in V(SC_1[n])} d(u)\epsilon(u) \\ &= 2 \times 3 \times (2n+3) + 4 \times 3 \times (2n+4) + 4 \times 2 \times (2 \times (2n+5)).\end{aligned}$$

By simplifying above expression, $\xi(SC_1[n])$ for core of nanocone, i.e. for $n = 0$, can be written as

$$\xi(SC_1[0]) = 68n + 146 = 146.$$

This completes the proof. □

Theorem 3.2. *The eccentric-connectivity index of nanocone $SC_1[n]$ for $n \geq 1$ and n even is given by*

$$\xi(SC_1[n]) = 36n^3 + 196n^2 + 290n + 146.$$

Proof. For the nanocone $SC_1[n]$ we use only one quadrant of $SC_1[n]$ by using the concept of symmetry, labeled in Figure 3. One representative from a set of vertices have taken having same size and distance and are labeled by $w, x, y, z, v_1^j, v_2^j, v_i^j, v_{j+2}^j$ for $1 \leq i \leq n$, and their requisite information is given in Table 1.

Using Table 1, ECI of $SC_1[n]$ for $n \geq 1$, is given by

$$\begin{aligned}\xi(SC_1[n]) &= \sum_{u \in V(SC_1[n])} d(u)\epsilon(u) \\ &= 2 \times 3 \times (2n+3) + 4 \times 3 \times [(2n+5) + (2n+4) + (2n+5)] + \\ &\quad +4 \times 3 \times 2 \times \sum_{j=1}^{n-1} \big(2n + 2j + 5) + 4 \times 2 \times 2 \times (2n + 2j + 5) \\ &\quad +4 \times 3 \times 2 \times \sum_{j=1}^{n} \big(2n + 2j + 4) + +4 \times 3 \times 2 \times \sum_{j=2}^{n-1} \sum_{i=3}^{j+1} \big(2n + 2j - i + 7) \\ &\quad +4 \times 2 \times 2 \times \sum_{i=2}^{\frac{n+2}{2}} \big(2n + 2j - 2i + 8) + 4 \times 3 \times 2 \times \sum_{i=2}^{\frac{n}{2}} \big(2n + 2j - 2i + 7) \\ &\quad +4 \times 3 \times \sum_{j=1}^{n} \big(2n + j + 5).\end{aligned}$$

By simplifying above expression, $\xi(SC_1[n])$ for n even can be written as

$$\xi(SC_1[n]) = 36n^3 + 196n^2 + 290n + 146.$$

This completes the proof. $\square$

Corollary 3.3. *The total-eccentricity index of $SC_1[n]$ nanocone for n even is given by*

$$\varsigma(SC_1[n]) = 12n^3 + 60n^2 + 2^{n(5n+11)} + 92n + 62.$$

Corollary 3.4. *The first Zagreb-eccentricity index of $SC_1[n]$ nanocone for n even is given by*

$$M_1^*(SC_1[n]) = 18n^6 - 48n^5 + 142n^4 + 752n^3 + 217n^2 + 128n + 1082.$$

Theorem 3.5. *The eccentric-connectivity index of nanocone $SC_1[n]$ for n odd is given by*

$$\xi(SC_1[n]) = 36n^3 + 196n^2 + 290n + 148.$$

Proof. Using same technique of symmetry and by using Table 1, ECI of $SC_1[n]$ for $n \geq 1$, can be written as.

$$\begin{aligned}
\xi(SC_1[n]) &= \sum_{u \in V(SC_1[n])} d(u)\epsilon(u) \\
&= 2 \times 3 \times (2n+3) + 4 \times 3 \times (2n+5) + (2n+4) + (2n+5) + \\
&\quad +4 \times 3 \times 2 \times \sum_{j=1}^{n-1} \big(2n+2j+5\big) + 4 \times 2 \times 2 \times (2n+2j+5) \\
&\quad +4 \times 3 \times 2 \times \sum_{j=1}^{n} \big(2n+2j+4\big) + 4 \times 3 \times 2 \times \sum_{j=2}^{n-1} \sum_{i=3}^{j+1} \big(2n+2j-i+7\big) \\
&\quad +4 \times 2 \times 2 \times \sum_{i=2}^{\frac{n+3}{2}-1} \big(2n+2j-2i+8\big) + 4 \times 3 \times 2 \times \sum_{i=2}^{\frac{n+3}{2}-1} \big(2n+2j-2i+7\big) \\
&\quad +4 \times 2 \times \sum_{j=1}^{n-1} \big(2n+j+5\big) + 4 \times 2 \times (3n+5).
\end{aligned}$$

After simplification, $\xi(SC_1[n])$ for n odd can be written as

$$\xi(SC_1[n]) = 36n^3 + 196n^2 + 290n + 148.$$

which completes the proof. $\square$

Corollary 3.6. *The total-eccentricity index of $SC_1[n]$ nanocone for n odd is given by*

$$\varsigma(SC_1[n]) = 12n^3 + 70n^2 + 114n + 62.$$

Corollary 3.7. *The first Zagreb-eccentricity index of $SC_1[n]$ nanocone for n odd is given by*

$$M_1^*(SC_1[n]) = 18n^6 - 48n^5 + 142n^4 + 692n^3 + 9n^2n + 6n + 1183.$$

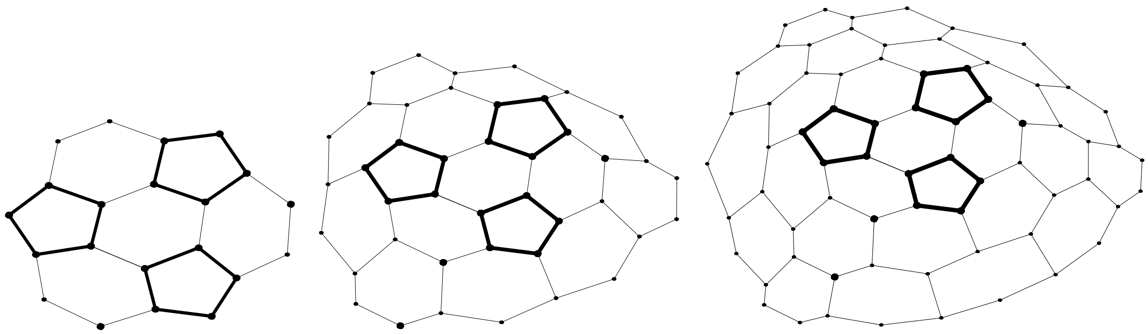

Figure 4: Representation of nanocone $SC_2[n]$ type with two growth stages.

4 Eccentric-connectivity (EC), total-eccentricity (TE) indices of nanocone $SC_2[n]$

In this section, we compute the EC and TE indices of the second type of nanocone $SC_2[n]$. The degrees and eccentricities of the core vertices of $SC_2[n]$ are shown in Table 2. The degrees and eccentricities of the vertices of $SC_2[n]$, $n \geq 1$, are given in Table 3 and Table 4.

$v \in V(G)$	$d(v)$	$\epsilon(v)$	f
a, b	3	$2n+5$	3
c, e, g	2	$2n+6$	3
d, f	3	$2n+6$	3

Table 2: The representatives of vertices of $SC_2[0]$ with their degrees, eccentricities and frequencies of occurrence.

Theorem 4.1. *The ECI of nanocone $SC_2[0]$ is given by*

$$\xi(SC_2[0]) = 306.$$

Proof. For the nanocone $SC_2[n]$ we use only one quadrant of $SC_2[n]$ by using the concept of symmetry, labeled in Figure 5. One representative from a set of vertices have been taken having same size and distance and are labeled by a, b, c, d, e, f, g for $1 \leq i \leq n$, also their requisite information is given in Table 2. Using Table 2, ECI of $SC_2[n]$ for $n \geq 1$, is given by

$$\begin{aligned} \xi(SC_2[n]) &= \sum_{u \in V(SC_2[n])} d(u)\epsilon(u) \\ &= 3 \times 3 \times (2n+5) + 3 \times 3 \times (2n+6) + 3 \times 2 \times (2n+6). \end{aligned}$$

After simplification, the eccentric-connectivity index $\xi(SC_2[0])$ can be written as:

$$\xi(SC_2[0]) = 108n + 306 = 306,$$

This completes the proof. □

Corollary 4.2. *The total-eccentricity and first Zagreb index of $SC_2[0]$ is given by*

$$\varsigma(SC_2[n]) = 42n + 120.$$

$$M_1^*(SC_2[n]) = 84n^2 + 480n + 690.$$

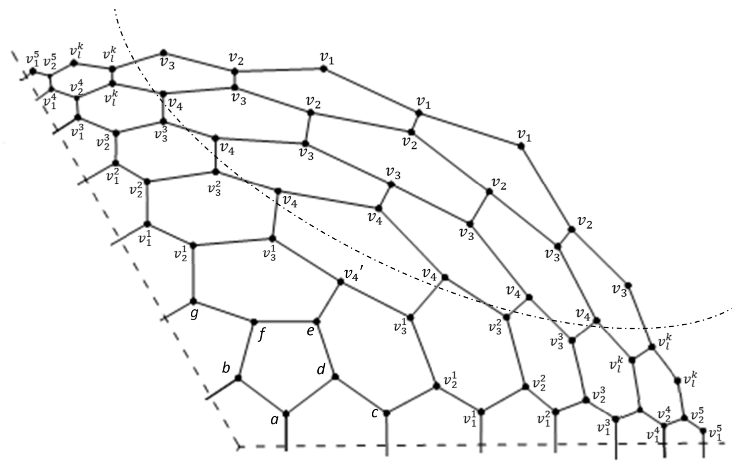

Figure 5: The nanocones $SC_2[5]$ with vertex labeling of a single quadrant. The vertices $v_i's$ in one quadrant are separated by a dashed line.

$v \in V(G)$	$d(v)$	$\epsilon(v)$	f
a, b	3	$2n+5$	3
c, d, e, f, g	3	$2n+6$	3
$v_1^j \quad (1 \leq j \leq r-1)$	3	$2n+6$	6
$v_1^j \quad (0 \leq j \leq n-r-1)$	3	$2n+2j+8$	6
$v_1^j \quad (j = n-r)$	2	$2n+2j+8$	6
$v_2^j \quad (1 \leq j \leq r)$	3	$2n+7$	6
$v_2^j \quad (1 \leq j \leq n-r)$	3	$2n+2j+7$	6
$v_3^j \quad (1 \leq j \leq r)$	3	$2n+8$	6
v_4'	3	$2n+9$	3
$v_i \quad (1 \leq i \leq \frac{n-1}{2})$	3	$3n-i+8$	$3 \times (2i+1)$
$v_i \quad (\frac{n+1}{2} \leq i \leq n-1 \text{ and } n \cong 1(mod4))$	3	$3n-i+8$	$3 \times (\frac{n+9}{2})$
$v_i \quad (\frac{n+1}{2} \leq i \leq n-1 \text{ and } n \cong 3(mod4))$	3	$3n-i+8$	$3 \times (\frac{n+11}{2})$
$v_i \quad (1 \leq i \leq \frac{n-1}{4} \text{ and } n \cong 1(mod4))$	2	$\frac{7n+9}{2} - 2i$	3
$v_i \quad (1 \leq i \leq \frac{n+1}{4} \text{ and } n \cong 3(mod4))$	2	$\frac{7n+9}{2} - 2i$	3
$v_l^k \quad (1 \leq k \leq \frac{n-5}{2} \text{ and } 1 \leq l \leq n-2k-1)$	3	$2n+l+k+7$	6
$v_l^k \quad (1 \leq k \leq \frac{n-5}{2} \text{ and } l = n-2k)$	2	$3n-k+7$	6
$v_l^k \quad (k = \frac{n-3}{2} \text{ and } l = 1)$	2	$\frac{5n}{2} + \frac{17}{2}$	6

Table 3: The representatives of vertices of $SC_2[n]$ for n odd with their degrees, eccentricities and frequencies of occurrence, for $1 \leq i \leq n$.

Theorem 4.3. *The eccentric-connectivity index of nanocone $SC_2[n]$ for n odd is given by*

$$\xi(SC_2[n]) = \begin{cases} \frac{6375}{16}n - \frac{375}{16} + \frac{375}{16}n^3 + \frac{2985}{16}n^2, & \textit{when } n \cong 1(mod4) \\ \frac{6663}{16}n - \frac{1119}{16} + \frac{375}{16}n^3 + \frac{3147}{16}n^2, & \textit{when } n \cong 3(mod4). \end{cases}$$

Proof. Using same concept of symmetry for nanocone $SC_2[n]$, only one branch of $SC_2[n]$ is used as labelled in Figure 4. One representative from a set of vertices have been taken which have same size and distances and are labelled by a, b, c, d, e, f, g and v_i^j for $1 \leq i \leq n$ as shown in Table 3. Using Table 3,

$v \in V(G)$	$d(v)$	$\epsilon(v)$	f
a, b	3	$2n+5$	1
c, d, e, f, g	3	$2n+6$	1
$v_1^j \quad (1 \leq j \leq r-1)$	3	$2n+6$	6
$v_1^j \quad (r \leq j \leq n-1)$	3	$2n+2j-2r+7$	6
$v_1^j \quad (j = n)$	2	$2n+2j-2r+7$	6
$v_2^j \quad (1 \leq j \leq r)$	3	$2n+7$	6
$v_2^j \quad (r+1 \leq j \leq n)$	3	$2n+2j-2r+6$	6
$v_3^j \quad (1 \leq j \leq r+1)$	3	$2n+8$	6
$v_i \quad (1 \leq i \leq \frac{n}{2}-1)$	3	$3n-i+8$	$3 \times (2i+1)$
$v_i \quad (\frac{n}{2} \leq i \leq n)$	3	$3n-i+8$	$3 \times (n+1)$
$v_i \quad (2 \leq i \leq \frac{n}{4}$ and $n \cong 0(mod4))$	2	$\frac{7n+9}{2}-2i$	3
$v_i \quad (2 \leq i \leq \frac{n-2}{4}$ and $n \cong 2(mod4))$	2	$\frac{7n+9}{2}-2i$	3
$v_l^k \quad (2 \leq k \leq \frac{n+2}{4}$ and $1 \leq l \leq n-4k+2)$	3	$2n+l+2k+6$	6
$v_l^k \quad (2 \leq k \leq \frac{n+2}{4}$ and $l = n-4k+3)$	2	$3n-2k+9$	6
$v_l^k \quad (1 \leq l \leq n-3$ and $k = 1)$	3	$2n+l+8$	6
$v_l^k \quad (l = n-2$ and $k = 1)$	2	$3n+6$	6

Table 4: The representatives of vertices of $SC_2[n]$ for n even with their degrees, eccentricities and frequencies of occurrence, for $1 \leq i \leq n$.

the eccentric-connectivity index of $SC_2[n]$ for $n \geq 1$, are computed in two cases. The eccentricities of v_i's with respective frequencies are presented in Table 3. It must be observed from Figure 5 that, when $n = 5$, the frequency of v_1 is 3, the frequency of v_2 is 5, and the frequency of v_3 and v_4 is 7. The eccentricities of these v_i's are presented in Table 3 and Table 4.

Case 1. When $n \cong 1(mod4)$.

$$\begin{aligned}
\xi(SC_2[n]) &= \sum_{u \in V(SC_2[n])} d(u)\epsilon(u) \\
&= 3 \times 3 \times [(2n+5)+(2n+5)+(2n+6)+(2n+6)+(2n+6)+(2n+6)+(2n+6)+(2n+6)] \\
&\quad +3 \times 3 \times 2 \times \sum_{j=1}^{r-1}(2n+6) + 3 \times 3 \times 2 \times \sum_{j=0}^{n-r-1}(2n+2j+8) + 3 \times 2 \times 2 \times \sum_{j=n-r}^{n-r}(2n+2j+8) \\
&\quad +3 \times 3 \times 2 \times \sum_{j=1}^{r}(2n+7) + 3 \times 3 \times 2 \times \sum_{j=1}^{n-r}(2n+2j+7) + 3 \times 3 \times 2 \times \sum_{j=1}^{r}(2n+8) \\
&\quad +3 \times 3 \times (2n+9) + 3 \times 3 \times [\sum_{i=1}^{\frac{n-1}{2}}(3n-i+8)(2i+1) + \sum_{i=\frac{n+1}{2}}^{n-1}(3n-i+8)(\frac{n+9}{2})] \\
&\quad -3 \times [2 \times \sum_{i=1}^{\frac{n-1}{4}}(\frac{7n+9}{2}-2i)] + 3 \times 3 \times 2 \times \sum_{k=1}^{\frac{n-5}{2}} \sum_{l=1}^{n-2k-1}(2n+l+k+7) \\
&\quad +3 \times 2 \times 2 \times \sum_{k=1}^{\frac{n-5}{2}}(3n-k+7) + 3 \times 2 \times 2 \times [\frac{5}{2}(n-1)+11].
\end{aligned}$$

After simplification, the eccentric-connectivity index $\xi(SC_2[n])$ can be written as:

$$\xi(SC_2[n]) = \frac{6375}{16}n - \frac{375}{16} + \frac{375}{16}n^3 + \frac{2985}{16}n^2.$$

Case 2. When $n \cong 3(mod 4)$.

$$\begin{aligned}
\xi(SC_2[n]) &= \sum_{u\in V(SC_2[n])} d(u)\epsilon(u) \\
&= 3\times 3\times[(2n+5)+(2n+5)+(2n+6)+(2n+6)+(2n+6)+(2n+6)+(2n+6)+(2n+6)] \\
&\quad +3\times 3\times 2\times\sum_{j=1}^{r-1}(2n+6)+3\times 3\times 2\times\sum_{j=0}^{n-r-1}(2n+2j+8)+3\times 2\times 2\times\sum_{j=n-r}^{n-r}(2n+2j+8) \\
&\quad +3\times 3\times 2\times\sum_{j=1}^{r}(2n+7)+3\times 3\times 2\times\sum_{j=1}^{n-r}(2n+2j+7)+3\times 3\times 2\times\sum_{j=1}^{r}(2n+8) \\
&\quad +3\times 3\times(2n+9)+3\times 3\times[\sum_{i=1}^{\frac{n-1}{2}}(3n-i+8)(2i+1)+\sum_{i=\frac{n+1}{2}}^{n-1}(3n-i+8)(\frac{n+11}{2})] \\
&\quad -3\times[2\times\sum_{i=1}^{\frac{n+1}{4}}(\frac{7n+9}{2}-2i)]+3\times 3\times 2\times\sum_{k=1}^{\frac{n-5}{2}}\sum_{l=1}^{n-2k-1}(2n+l+k+7) \\
&\quad +3\times 2\times 2\times\sum_{k=1}^{\frac{n-5}{2}}(3n-k+7)+3\times 2\times 2\times[\frac{5}{2}(n-1)+11].
\end{aligned}$$

After simplification, the eccentric-connectivity index $\xi(SC_2[n])$ can be written as:

$$\xi(SC_2[n]) = \frac{6663}{16}n - \frac{1119}{16} + \frac{375}{16}n^3 + \frac{3147}{16}n^2.$$

This completes the second case of the proof. □

Corollary 4.4. *The total-eccentricity index of $SC_2[n]$ nonocone for n odd is given by*

$$\varsigma(SC_2[n]) = \begin{cases} \frac{2203}{16}n - \frac{57}{4} + \frac{119}{16}n^3 + \frac{513}{8}n^2, & \textit{when } n \cong 1(mod4) \\ \frac{2275}{16}n - \frac{255}{8} + \frac{119}{16}n^3 + \frac{135}{2}n^2, & \textit{when } n \cong 3(mod4). \end{cases}$$

Corollary 4.5. *The first Zagreb index of $SC_2[n]$ nonocone for n odd is given by*

$$M_1^*(SC_2[n]) = \begin{cases} \frac{88971}{32}n + \frac{631905}{128} + \frac{225}{64}n^4 + \frac{963}{256}n^6 + \frac{273}{64}n^5 + \frac{15039}{64}n^3 + \frac{224607}{256}n^2, & \textit{when } n \cong 1(mod4) \\ \frac{399825}{128}n + \frac{296937}{64} - \frac{3033}{128}n^4 + \frac{963}{256}n^6 + \frac{303}{128}n^5 + \frac{4437}{32}n^3 + \frac{236787}{256}n^2, & \textit{when } n \cong 3(mod4). \end{cases}$$

Theorem 4.6. *The eccentric-connectivity index of nanocone $SC_2[n]$ for n even is given by*

$$\xi(SC_2[n]) = \begin{cases} 345 + \frac{2151}{4}n + \frac{87}{4}n^3 + \frac{819}{4}n^2, & \textit{when } n \cong 0(mod4) \\ 357 + \frac{2187}{4}n + \frac{87}{4}n^3 + \frac{819}{4}n^2, & \textit{when } n \cong 2(mod4). \end{cases}$$

Proof. Using symmetry of the nanocone $SC_2[n]$ we use only one branch of $SC_2[n]$ as labelled in Figure 5. One representative from a set of vertices have been taken having same size and distances, labelled by a, b, c, d, e, f, g and v_i^j for $1 \leq i \leq n$, given in Table 4.

Using Table 3, the ECI of $SC_2[n]$ for $n \geq 1$, can be written as follows.

Case 1. When $n \cong 0(mod4)$.

$$\begin{aligned}
\xi(SC_2[n]) &= \sum_{u \in V(SC_2[n])} d(u)\epsilon(u) \\
&= 3 \times 3 \times [(2n+5) + (2n+5) + (2n+6) + (2n+6) + (2n+6) + (2n+6) + (2n+6) + (2n+6)] \\
&\quad +3 \times 3 \times 2 \times \sum_{j=1}^{r-1}(2n+6) + 3 \times 3 \times 2 \times \sum_{j=r}^{n-1}(2n+2j-2r+7) + 3 \times 2 \times 2 \times \sum_{j=n}^{n}(2n+2j-2r+7) \\
&\quad +3 \times 3 \times 2 \times \sum_{j=1}^{r}(2n+7) + 3 \times 3 \times 2 \times \sum_{j=r+1}^{n}(2n+2j-2r+6) + 3 \times 3 \times 2 \times \sum_{j=1}^{r+1}(2n+8) \\
&\quad +3 \times 3 \times [\sum_{i=1}^{\frac{n}{2}-1}(3n-i+8)(2i+1) + \sum_{i=\frac{n}{2}}^{n}(3n-i+8)(n+1)] \\
&\quad -3 \times [2 \times \sum_{i=2}^{\frac{n}{4}}(\frac{7n+9}{2} - 2i) + (\frac{7n+9}{2} - 2)] + 3 \times 3 \times 2 \times \sum_{k=2}^{\frac{n+2}{4}} \sum_{l=1}^{n-4k+2}(2n+l+2k+6) \\
&\quad +3 \times 2 \times 2 \times \sum_{k=2}^{\frac{n+2}{4}}(3n-2k+9) + 3 \times 3 \times 2 \times \sum_{l=1}^{n-3}(2n+l+8) + 3 \times 2 \times 2 \times (3n+6).
\end{aligned}$$

After simplification, the eccentric-connectivity index $\xi(SC_2[n])$ can be written as:

$$\xi(SC_2[n]) = 345 + \frac{2151}{4}n + \frac{87}{4}n^3 + \frac{819}{4}n^2.$$

Case 2. When $n \cong 2(mod4)$.

$$\begin{aligned}
\xi(SC_2[n]) &= \sum_{u \in V(SC_2[n])} d(u)\epsilon(u) \\
&= 3 \times 3 \times [(2n+5) + (2n+5) + (2n+6) + (2n+6) + (2n+6) + (2n+6) + (2n+6) + (2n+6)] \\
&\quad +3 \times 3 \times 2 \times \sum_{j=1}^{r-1}(2n+6) + 3 \times 3 \times 2 \times \sum_{j=r}^{n-1}(2n+2j-2r+7) + 3 \times 2 \times 2 \times \sum_{j=n}^{n}(2n+2j-2r+7) \\
&\quad +3 \times 3 \times 2 \times \sum_{j=1}^{r}(2n+7) + 3 \times 3 \times 2 \times \sum_{j=r+1}^{n}(2n+2j-2r+6) + 3 \times 3 \times 2 \times \sum_{j=1}^{r+1}(2n+8) \\
&\quad +3 \times 3 \times [\sum_{i=1}^{\frac{n}{2}-1}(3n-i+8)(2i+1) + \sum_{i=\frac{n}{2}}^{n}(3n-i+8)(n+1)] \\
&\quad -3 \times [2 \times \sum_{i=2}^{\frac{n-2}{4}}(\frac{7n+9}{2} - 2i) + (\frac{7n+9}{2} - 2)] + 3 \times 3 \times 2 \times \sum_{k=2}^{\frac{n+2}{4}} \sum_{l=1}^{n-4k+2}(2n+l+2k+6) \\
&\quad +3 \times 2 \times 2 \times \sum_{k=2}^{\frac{n+2}{4}}(3n-2k+9) + 3 \times 3 \times 2 \times \sum_{l=1}^{n-3}(2n+l+8) + 3 \times 2 \times 2 \times (3n+6).
\end{aligned}$$

After simplification, the eccentric-connectivity index $\xi(SC_2[n])$ can be written as:

$$\xi(SC_2[n]) = 357 + \frac{2187}{4}n + \frac{87}{4}n^3 + \frac{819}{4}n^2.$$

This completes the second case of proof. $\square$

Corollary 4.7. *The total-eccentricity index of $SC_2[n]$ nonocone for n odd is given by*

$$\varsigma(SC_2[n]) = \begin{cases} 132 + \frac{1499}{8}n + \frac{29}{4}n^3 + \frac{1101}{16}n^2, & \text{when } n \cong 0(mod4) \\ 138 + \frac{1535}{8}n + \frac{29}{4}n^3 + \frac{1101}{16}n^2, & \text{when } n \cong 2(mod4). \end{cases}$$

Corollary 4.8. *The first Zagreb index of $SC_2[n]$ nonocone for n even is given by*

$$M_1^*(SC_2[n]) = \begin{cases} 1710n + \frac{21075}{4} + \frac{53085}{256}n^4 + \frac{999}{256}n^6 + \frac{3009}{128}n^5 + \frac{47517}{64}n^3 + \frac{43629}{64}n^2, & \text{when } n \cong 0(mod4) \\ \frac{3405}{2}n + \frac{21027}{4} + \frac{53085}{256}n^4 + \frac{999}{256}n^6 + \frac{3009}{128}n^5 + \frac{47985}{64}n^3 + \frac{44325}{64}n^2, & \text{when } n \cong 2(mod4). \end{cases}$$

5 Conclusion

In this paper, two families of nanocones are considered and their eccentric-connectivity index, total-eccentricity index and eccentricity-based Zagreb index are computed. In future, we are interested to formulate the architectures of next complex structured nanocones with more pentagons at the tip of cones [8] and study their topological invariants which could be quite helpful to understand their chemical structure and behavior.

References

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

[2] Mian Muhammad Zobair, Mehar Ali Malik, Hani Shaker, Noor Rehman, Eccentricity based topological invariants of triangulane dendrimers. Utilitas Mathematica. **107** (2018) 193–206.

[3] Mian Muhammad Zobair, Hani Shaker, Muhammad Imran, Noor Rehman, Polynomial structure of Benzene ring embedded in periodic-type surface in 2-dimension. Utilitas Mathematica. **108** (2018) 253–263.

[4] H. Hosoya, Topological Index. A Newly Proposed Quantity Characterizing the Topological Nature of Structural Isomers of Saturated Hydrocarbons, Bull. Chem. Soc. Japan. **44** (1971) 2322-2239.

[5] S. Bajaj, S.S. Sambi, A.K. Madan, Topological models for prediction of anti-HIV activity of acylthiocarbamates, Bioorganic & Medicinal Chemistry, **13** (2005) 3263-3268.

[6] S. Bajaj, S.S. Sambi, S. Gupta, A.K. Madan, Model for prediction of anti-HIV activity of 2-pyridinone derivatives using novel topological descriptor, QSAR & Combinatorial Science, **25** (2006) 813-823.

[7] M. Saheli, H. Saati, A. R. Ashrafi, The eccentric connectivity index of one pentagonal carbon nanocones, OAM-RC **4(6)**, 2010, 896 – 897.

[8] H. Heiberg Andersen, G. Helgesen and K. Knudsen, Nanocones - a different form of carbon with unique properties, Materials Research Society. **901E**, s34.1- 34.8 (2006).

[9] Wei Gao and Mohammad Reza Farahani On topological indices of poly oxide, poly silicate, DOX, and DSL networks, Journal of Nanotechnology. **6** (2016).

[10] M. Ghorbani, M.A. Hosseinzadeh, A new version of Zagreb indices, Filomat, **26**(1), 93-100 (2012).

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

[12] A. Madanshekaf, M. Ghaneei, The second-order connectivity index of dendrimer nanostars, Digest J. Nanomater. Biostruct. **6**, 433-437 (2011).

[13] M. Rostami, M. Shabanian, H. Moghanian, Some topological indices for theoretical study of two types of nanostar dendrimers, Digest J. Nanomater. Biostruct. **7**(1), 247–252 (2012).

[14] D. Vukičević, B. Furtula, On Van Degrees of Vertices and Van Indices of Graphs, J. Math. Chem. **46**, 13–69 (2009).

[15] A. Khaksar, M. Ghorbani , H. R. Maimani, On atom bond connectivity and GA indices of nanocones, Optoelectronics and Advanced Materials – Rapid Communications, **4 (11)**, 1868-1870 (2010).