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Various F-Sombor Leap Indices and Reduced Sombor Leap Index of Some Special Graphs and Circumcoronene Series of Benzenoid

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Abstract. In chemical graph theory, many researchers have proved that connection-based versions of some degree-based topological indices have shown better results than their respective degree-based ones. The connection-based indices are also known as leap indices. Currently, there are many degree-based topological indices of which connection-based versions have neither been formulated nor explored. Hence, in this paper, various novel leap indices of existing degree-based indices are introduced and mathematical closed-form expressions of these indices are formulated for path, cycle, and some special graphs. As an application, these indices are calculated for a particular series of the Benzenoid structure to study their characteristic trend.

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1 Introduction

$G(V, E)$ is a graph with $|V| = n$ vertices and $|E| = m$ edges such that each edge in E is adjacent to a pair of vertices in V. The distance $d(u, v)$ between any pair of vertices 'u' and 'v' in G is the number of edges involved in the shortest path between them. The number of vertices at a distance '2' from a vertex 'u' is called the connection number of 'u' and is denoted by $d_2(u)$. The topological indices formulated based on connection numbers are called leap indices.

A topological index is a graph-invariant number that is inferred from a chemical graph, a graph representing a molecule. The chemical graph is obtained by considering atoms of the molecule as vertices and bonds between them as edges. Here, we focus on simple graphs depending on the definition of a chemical graph[19]. The first topological index was introduced by Harry Wiener in 1947 to calculate the boiling points of paraffin. Since then, more than 3000 topological indices have been introduced and are being calculated using various chemical databases.

A molecular descriptor is a function that converts the chemical information encoded in a molecule to a numerical value. Topological indices are the 2-D molecular descriptors that play a major role in a branch known as Mathematical Chemistry. Using these mathematical values, it is possible to investigate the molecules' physicochemical properties, bioactivity, and even toxicity. This is done by analyzing the regression models such as Quantitative Structure-Property Relationship(QSPR), Quantitative Structure-Activity Relationship(QSAR), and Quantitative Structure-Toxicity Relationship(QSTR). This regression analysis gives a reasonable basis for the mathematical correlation between the properties and the topological index. The QSPR/QSAR analysis has proved their ability in pharmacology (drug design), medicinal chemistry, environmental sciences, etc.[10] and [20]. In drug design, it is possible to find the lead, most favorable, and desired compounds from millions of untested compounds by predicting their properties using these analyses. These models serve as the cheapest alternative for time-consuming and expensive laboratory experiments in reactivity and stability studies. Not only in studying various molecular properties, these topological indices are also used in investigating the structural characteristics of various nanostructures.

Many researchers have introduced different versions of existing topological indices. Hence, the broad classification of indices is degree-based, distance-based, spectrum-based, and neighborhood-based topological indices. The connection-based or leap indices are also distance-based indices as they are formulated using the cardinality of vertices at a distance 2. Here, most leap indices are formulated by replacing the degree of the vertex in a degree-based topological index with a connection number. A lot of work has been done on these leap indices of special and general graphs too. For more details, refer to [1], [6], [12], [16], [17], and [18]. However, many more degree-based indices are not explored in terms of connection numbers. We consider such indices to be explored in detail.

In this paper, to the best of our knowledge and literature review, we consider some degree-based indices F-Sombor, modified F-Sombor, and reduced Sombor index for which the connection-based versions are not formulated. We introduce connection-based versions of the above indices and also formulate a new degree-based index, second F-Sombor index, and its connection-based version. In [13], Kulli determined the connection variants of F-index and F_1 index as F-leap and F_1-leap indices as follows:

$$FL(G) = \sum_{u \in V(G)} d_2^3(u) \quad and \quad F_1L(G) = \sum_{uv \in E(G)} d_2^2(u) + d_2^2(v).$$

Later, Kulli et al. also formulated and calculated Sombor and modified Sombor leap indices for some chemical drugs [15].

$$SL(G) = \sum_{uv \in E(G)} \sqrt{d_2^2(u) + d_2^2(v)} \quad and$$

$$^{m}SL(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_2^2(u) + d_2^2(v)}}.$$

He then introduced F-Sombor and modified F-Sombor index in [14]. These are defined as follows:

$$FSO(G) = \sum_{uv \in E(G)} \sqrt{(d_G^2(u))^2 + (d_G^2(v))^2} \quad and$$

$$^{m}FSO(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{(d_G^2(u))^2 + (d_G^2(v))^2}}.$$

Gutman [11] introduced a degree-based descriptor namely reduced Sombor index as

$$SO_{red}(G) = \sum_{uv\in E(G)} \sqrt{(d_G(u)-1)^2 + (d_G(v)-1)^2}.$$

Here, we introduce the connection-based versions of indices mentioned above as F-Sombor leap index, modified F-Sombor leap index, and reduced Sombor leap index as

$$FSO_L(G) = \sum_{uv\in E(G)} \sqrt{(d_2^2(u))^2 + (d_2^2(v))^2}\,,$$

$$^{m}FSO_L(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{(d_2^2(u))^2 + (d_2^2(v))^2}},$$

$$^{red}SO_L(G) = \sum_{uv\in E(G)} \sqrt{(d_2(u)-1)^2 + (d_2(v)-1)^2}.$$

We also put forth a degree-based index, namely Second F-Sombor index and its leap version Second F-Sombor leap index as

$$^{2}FSO(G) = \sum_{uv\in E(G)} (d_G^2(u))^2 \times (d_G^2(v))^2,$$

$$^{2}FSO_L(G) = \sum_{uv\in E(G)} (d_2^2(u))^2 \times (d_2^2(v))^2.$$

The mathematical closed-form expressions of the aforementioned novel leap indices are formulated for path, cycle, and special graphs like wheel, windmill, and friendship graph in the next section.

2 Results

Definition 2.1. *The path P_n of length 'n-1' is a sequence of distinct 'n' vertices such that each pair of vertices (u, v) is an edge of the graph. In other words, P_n has $|V| = n$ and $|E| = n - 1$.*

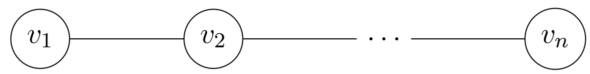


Figure 1: Path(P_n).

Lemma 2.2. *Let P_n be a path of length 'n-1' on 'n' nodes(as shown in Figure 1). Then, for $n \geq 5$, the connection number '$d_2(u)$' is as follows:*
$d_2(v_i) = 2; 3 \leq i \leq n-2$ *and*
$d_2(v_i) = 1;$ *otherwise.*

Theorem 2.3. *If P_n is a path on $n \geq 5$ vertices, then*

(i) $FSO_L(P_n) = 4\sqrt{2}n - 17.2096,$

(ii) ${}^{m}FSO_L(P_n) = \frac{1}{4\sqrt{2}}n + 1.1054,$

(iii) ${}^{red}SO_L(P_n) = \sqrt{2}n - 5.0710,$

(iv) ${}^{2}FSO_L(P_n) = 256n - 1246.$

Proof. Let P_n be a path on 'n' vertices, $n \geq 5$. Using Lemma 2.2, edge partition of the path P_n can be done based on the connection number as
$E_1 = \{v_iv_j \in E(P_n) \mid d_2(v_i) = 1, d_2(v_j) = 1\},$
$E_2 = \{v_iv_j \in E(P_n) \mid d_2(v_i) = 1, d_2(v_j) = 2\},$
$E_3 = \{v_iv_j \in E(P_n) \mid d_2(v_i) = 2, d_2(v_j) = 2\}.$
From Figure 1,
$\mid E_1 \mid = 2$, $\mid E_2 \mid = 2$, and $\mid E_3 \mid = n-5$.

(i) Using the definition of $FSO_L(G)$,

$$FSO_L(P_n) = \sum_{uv \in E_1} \sqrt{1^4 + 1^4} + \sum_{uv \in E_2} \sqrt{1^4 + 2^4} + \sum_{uv \in E_3} \sqrt{2^4 + 2^4}$$
$$= 2\sqrt{2} + 2\sqrt{17} + (n-5)\sqrt{32} = 4\sqrt{2}n - 17.2096.$$

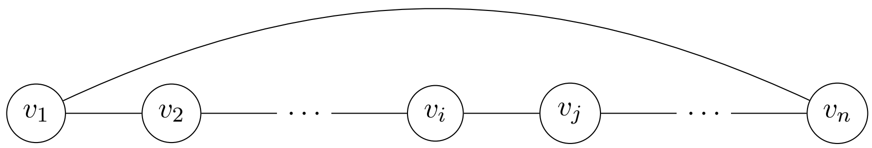


Figure 2: Cycle(C_n).

(ii) Using the definition of ${}^{m}FSO_L(G)$,

$$\begin{aligned}{}^{m}FSO_L(P_n) &= \sum_{uv\in E_1}\frac{1}{\sqrt{1^4+1^4}} + \sum_{uv\in E_2}\frac{1}{\sqrt{1^4+2^4}} + \sum_{uv\in E_3}\frac{1}{\sqrt{2^4+2^4}}\\ &= \frac{2}{\sqrt{2}} + \frac{2}{\sqrt{17}} + \frac{n-5}{\sqrt{32}} = \frac{1}{4\sqrt{2}}n + 1.0154.\end{aligned}$$

(iii) From the definition of ${}^{red}SO_L(G)$,

$$\begin{aligned}{}^{red}SO_L(P_n) = &\sum_{uv\in E_1}\sqrt{(1-1)^2+(1-1)^2} +\\ &\sum_{uv\in E_2}\sqrt{(1-1)^2+(2-1)^2} + \sum_{uv\in E_3}\sqrt{(2-1)^2+(2-1)^2}\\ =&0+2+(n-5)\sqrt{2} = \sqrt{2}n - 5.0710.\end{aligned}$$

(iv) From the definition of ${}^{2}FSO_L(G)$,

$$\begin{aligned}{}^{2}FSO_L(P_n) &= \sum_{uv\in E_1}1^4\times1^4 + \sum_{uv\in E_2}1^4\times2^4 + \sum_{uv\in E_3}2^4\times2^4\\ &=2+32+(n-5)256 = 256n-1246. \quad\square\end{aligned}$$

Definition 2.4. *A cycle C_n is a path on a finite sequence of '$n \geq 3$' vertices that starts at any vertex, v_i, and ends at the same vertex.*

Lemma 2.5. *Let C_n be a cycle on 'n' vertices of length 'n' as shown in Figure 2. Then, for $n \geq 5$, we have $d_2(v_i) = 2, \forall v_i \in V(C_n)$.*

Theorem 2.6. *For a cycle C_n with $n \geq 5$,*

(i) $FSO_L(C_n) = 4\sqrt{2}n$,

(ii) ${}^{m}FSO_L(C_n) = \frac{\sqrt{2}}{8}n$,

(iii) ${}^{red}SO_L(C_n) = \sqrt{2}n$,

(iv) ${}^{2}FSO_L(C_n) = 256n$.

Proof. Let C_n be a cycle with '$n \geq 5$' vertices. From Lemma 2.5, the edge set can be $E_1 = \{v_iv_j \in E(C_n) \mid d_2(v_i) = 2\}$. From Figure 2, it is clear that $\mid E_1 \mid = n$.

(i) From the definition of $FSO_L(G)$,

$$FSO_L(C_n) = \sum_{uv \in E_1} \sqrt{2^4 + 2^4} = 4\sqrt{2}n.$$

(ii) Using the definition of ${}^{m}FSO_L(G)$,

$${}^{m}FSO_L(C_n) = \sum_{uv \in E_1} \frac{1}{\sqrt{2^4 + 2^4}} = \frac{n}{4\sqrt{2}}.$$

(iii) From the definition of ${}^{red}SO_L(G)$,

$${}^{red}SO_L(C_n) = \sum_{uv \in E_1} \sqrt{(2-1)^2 + (2-1)^2} = \sqrt{2}n.$$

(iv) From the definition of ${}^{2}FSO_L(G)$,

$${}^{2}FSO_L(C_n) = \sum_{uv \in E_1} 2^4 \times 2^4 = 256n. \quad \square$$

Definition 2.7. *The wheel $W_n (n \geq 3)$ is a join of a cycle C_n with '$n \geq 3$' vertices and complete graph K_1. The Vertex of K_1 is called apex and the rest 'n' vertices of C_n are known as rim vertices. W_n has '$n+1$' vertices and '$2n$' edges.*

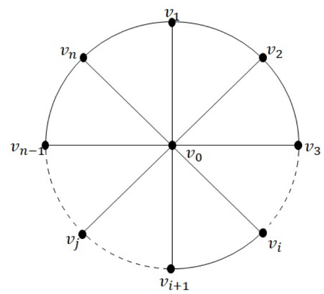


Figure 3: Wheel (W_n).

Lemma 2.8. *If W_n is a wheel with $n \geq 3$ as shown in Figure 3, then $d_2(v_0) = 0$, where $v_0 \in V(K_1)$ and $d_2(v_i) = n - 3$, where $v_i \in V(C_n)$.*

Theorem 2.9. *If W_n is a wheel on $n \geq 4$ vertices, then*

(i) $FSO_L(W_n) = 2.4142n(n-3)^2$,

(ii) ${}^{m}FSO_L(W_n) = \frac{n}{(n-3)^2}\left[1 + \frac{1}{\sqrt{2}}\right]$,

(iii) ${}^{red}SO_L(W_n) = n\sqrt{1 + (n-4)^2} + \sqrt{2}n(n-4)$,

(iv) ${}^{2}FSO_L(W_n) = n(n-3)^8$.

Proof. Let W_n be a wheel with 'n' vertices such that $n \geq 4$. Using Lemma 2.8 and Figure 3, edge partition of W_n can be done as follows:

$E_1 = \{v_0 v_i \in E(W_n) \mid d_2(v_0) = 0, d_2(v_i) = n - 3\}$,
$E_2 = \{v_i v_j \in E(W_n) \mid d_2(v_i) = n - 3, \forall i\}$.
Then $\mid E_1 \mid = n$ and $\mid E_2 \mid = n$.

(i) Using the definition of $FSO_L(G)$,

$$FSO_L(W_n) = \sum_{uv \in E_1} \sqrt{0^4 + (n-3)^4} + \sum_{uv \in E_2} \sqrt{(n-3)^4 + (n-3)^4}$$
$$= n(n-3)^2 + n\sqrt{2}(n-3)^2 = 2.4142n(n-3)^2.$$

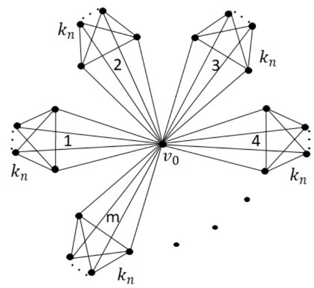


Figure 4: Windmill Graph(W_n^m).

(ii) Using the definition of ${}^{m}FSO_L(G)$,

$$
\begin{aligned}
{}^{m}FSO_L(W_n) &= \sum_{uv\in E_1} \frac{1}{\sqrt{(n-3)^4}} + \sum_{uv\in E_2} \frac{1}{\sqrt{2(n-3)^4}} \\
&= \frac{n}{(n-3)^2} + \frac{n}{\sqrt{2}(n-3)^2} = \frac{n}{(n-3)^2}\left[1+\frac{1}{\sqrt{2}}\right].
\end{aligned}
$$

(iii) From the definition of ${}^{red}SO_L(G)$,

$$
\begin{aligned}
{}^{red}SO_L(W_n) &= \sum_{uv\in E_1} \sqrt{(0-1)^2+(n-3-1)^2} + \\
&\quad \sum_{uv\in E_2} \sqrt{(n-3-1)^2+(n-3-1)^2} \\
&= n\sqrt{1+(n-4)^2} + \sqrt{2}n(n-4).
\end{aligned}
$$

(iv) From the definition of ${}^{2}FSO_L(G)$,

$$
\begin{aligned}
{}^{2}FSO_L(W_n) &= \sum_{uv\in E_1} 0^4 \times (n-3)^4 + \sum_{uv\in E_2} (n-3)^4 \times (n-3)^4 \\
&= n(n-3)^8. \quad \square
\end{aligned}
$$

Definition 2.10. *'$m \geq 2$' copies of a complete graph K_n, '$n \geq 2$' with a vertex in common form a graph known as the French windmill graph or the windmill graph. It is denoted as W_n^m. Here, $\mid V(W_n^m) \mid = m(n-1)+1$ and $\mid E(W_n^m) \mid = \frac{mn(n-1)}{2}$.*

Lemma 2.11. *Let W_n^m be a windmill graph such that $m \geq 2$ and $n \geq 3$ as shown in Figure 4. Then $d_2(v_0) = 0$, where v_0 is the central vertex and $d_2(v_i) = (m-1)(n-1)$, where $v_i \in V(W_n^m) - \{v_0\}$.*

Theorem 2.12. *If W_n^m is a windmill graph with $m \geq 2$ and $n \geq 3$, then*

(i) $FSO_L(W_n^m) = m(m-1)^2(n-1)^3\left(1 + \frac{n-2}{\sqrt{2}}\right)$,

(ii) ${}^{m}FSO_L(W_n^m) = \frac{m}{(m-1)^2(n-1)}\left(1 + \frac{n-2}{2\sqrt{2}}\right)$,

(iii) ${}^{red}SO_L(W_n^m) = m(n-1)\left(\sqrt{1+(mn-m-n)^2} + \frac{n-2}{\sqrt{2}}(mn-m-n)\right)$,

(iv) ${}^{2}FSO_L(W_n^m) = \frac{m(n-2)(m-1)^8(n-1)^9}{2}$.

Proof. Let W_n^m be a windmill graph having '$m(n-1)+1$' vertices and '$m[\frac{n(n-1)}{2}]$' edges such that $m \geq 2$ and $n \geq 3$. Let 'v_0' be the central vertex as shown in Figure 4. Using Lemma 2.11, edge partition of W_n^m will be as follows:

$E_1 = \{v_0v_i \in E(W_n^m) \mid d_2(v_0) = 0, d_2(v_i) = (m-1)(n-1)\}$,
$E_2 = \{v_iv_j \in E(W_n^m) \mid d_2(v_i) = (m-1)(n-1), \forall i\}$.
Then, $\mid E_1 \mid = m(n-1)$ and $\mid E_2 \mid = \frac{m(n-1)(n-2)}{2}$.

(i) Using the definition of $FSO_L(G)$,

$$\begin{aligned} FSO_L(W_n^m) = &\sum_{uv\in E_1} \sqrt{0+(m-1)^4(n-1)^4} + \\ &\sum_{uv\in E_2} \sqrt{(m-1)^4(n-1)^4+(m-1)^4(n-1)^4} \\ =&m(n-1)(m-1)^2(n-1)^2 + \\ &\frac{m(n-1)(n-2)\sqrt{2}(m-1)^2(n-1)^2}{2} \\ =&m(m-1)^2(n-1)^3\left[1+\frac{n-2}{\sqrt{2}}\right]. \end{aligned}$$

(ii) Using the definition of ${}^{m}FSO_L(G)$,

$$\begin{aligned}
{}^{m}FSO_L(W_n^m) &= \sum_{uv\in E_1} \frac{1}{\sqrt{(m-1)^4(n-1)^4}} + \sum_{uv\in E_2} \frac{1}{\sqrt{2(m-1)^4(n-1)^4}} \\
&= \frac{m(n-1)}{(m-1)^2(n-1)^2} + \frac{m(n-1)(n-2)}{2\sqrt{2}(m-1)^2(n-1)^2} \\
&= \frac{m}{(n-1)(m-1)^2}\left[1 + \frac{n-2}{2\sqrt{2}}\right].
\end{aligned}$$

(iii) From the definition of ${}^{red}SO_L(G)$,

$$\begin{aligned}
{}^{red}SO_L(W_n^m) &= \sum_{uv\in E_1} \sqrt{(-1)^2 + ((m-1)(n-1)-1)^2} + \\
&\quad \sum_{uv\in E_2} \sqrt{2[(m-1)(n-1)-1]^2} \\
&= m(n-1)\sqrt{1+(mn-m-n)^2} + \\
&\quad \frac{m(n-1)(n-2)}{2}\sqrt{2}(mn-m-n) \\
&= m(n-1)\left[\sqrt{1+(mn-m-n)^2} + \frac{n-2}{\sqrt{2}}(mn-m-n)\right].
\end{aligned}$$

(iv) From the definition of ${}^{2}FSO_L(G)$,

$$\begin{aligned}
{}^{2}FSO_L(W_n^m) &= \sum_{uv\in E_1} 0^4 \times (m-1)^4(n-1)^4 + \sum_{uv\in E_2} [(m-1)^4(n-1)^4]^2 \\
&= \frac{m(n-1)(n-2)}{2} \times (m-1)^8(n-1)^8 \\
&= \frac{m(n-2)(m-1)^8(n-1)^9}{2}. \quad \square
\end{aligned}$$

Definition 2.13. *The graph formed by 'n' copies of a cycle C_3 with a common vertex is known as a friendship graph. It is denoted by $F_3^{(n)}$. The common vertex is referred to as the central vertex. Clearly, $F_3^{(n)}$ has 2n+1 vertices and 3n edges.*

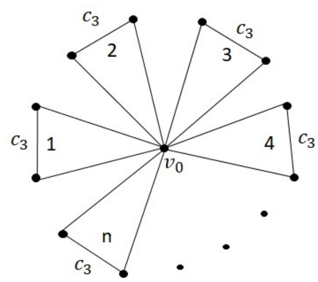


Figure 5: Friendship Graph($F_3^{(n)}$).

Lemma 2.14. *Let $F_3^{(n)}$ be a friendship graph with vertices labeled as shown in Figure 5. Then $d_2(v_0) = 0$, where v_0 is the common vertex and $d_2(v_i) = 2n - 2, \forall v_i \in V(F_3^{(n)}) - \{v_0\}$.*

Theorem 2.15. *If $F_3^{(n)}$ is a friendship graph with $n \geq 2$, then*

(i) $FSO_L(F_3^{(n)}) = 4n(n-1)^2[2+\sqrt{2}]$,

(ii) ${}^{m}FSO_L(F_3^{(n)}) = \frac{n}{4(n-1)^2}\left[2+\frac{1}{\sqrt{2}}\right]$,

(iii) ${}^{red}SO_L(F_3^{(n)}) = 2n\sqrt{1+(2n-3)^2} + \sqrt{2}n(2n-3)$,

(iv) ${}^{2}FSO_L(F_3^{(n)}) = 256n(n-1)^8$.

Proof. Let $F_3^{(n)}$ be a Friendship graph having '2n+1' vertices and '3n' edges such that $n \geq 2$. Consider 'v_0' to be the central vertex as shown in Figure 5. Using Lemma 2.14, edge partition of $F_3^{(n)}$ will be as follows

$E_1 = \{v_0v_i \in E(F_3^{(n)}) \mid d_2(v_0) = 0, d_2(v_i) = 2n-2\}$,
$E_2 = \{v_iv_j \in E(F_3^{(n)}) \mid d_2(v_i) = 2n-2, \forall i\}$.
Then $\mid E_1 \mid = 2n$ and $\mid E_2 \mid = n$.

(i) Using the definition of $FSO_L(G)$,

$$FSO_L(F_3^{(n)}) = \sum_{uv\in E_1}\sqrt{0^4+(2n-2)^4} + \sum_{uv\in E_2}\sqrt{2\times(2n-2)^4}$$
$$= 8n(n-1)^2 + 4\sqrt{2}n(n-1)^2 = 4n(n-1)^2[2+\sqrt{2}].$$

(ii) Using the definition of ${}^{m}FSO_L(G)$,

$$
\begin{aligned}
{}^{m}FSO_L(F_3^{(n)}) &= \sum_{uv\in E_1} \frac{1}{\sqrt{(0)^4+(2n-2)^4}} + \sum_{uv\in E_2} \frac{1}{\sqrt{2\times(2n-2)^4}} \\
&= \frac{2n}{(2n-2)^2} + \frac{n}{\sqrt{2}(2n-2)^2} = \frac{n}{4(n-1)^2}\left[2+\frac{1}{\sqrt{2}}\right].
\end{aligned}
$$

(iii) From the definition of ${}^{red}SO_L(G)$,

$$
\begin{aligned}
{}^{red}SO_L(F_3^{(n)}) &= \sum_{uv\in E_1} \sqrt{(-1)^2+(2n-2-1)^2} + \sum_{uv\in E_2} \sqrt{2(2n-3)^2} \\
&= 2n\sqrt{1+(2n-3)^2} + \sqrt{2}n(2n-3).
\end{aligned}
$$

(iv) From the definition of ${}^{2}FSO_L(G)$,

$$
\begin{aligned}
{}^{2}FSO_L(F_3^{(n)}) &= \sum_{uv\in E_1} (0)^4(2n-2)^4 + \sum_{uv\in E_2} (2n-2)^4(2n-2)^4 \\
&= n\times 2^8(n-1)^8 = 256n(n-1)^8. \quad \square
\end{aligned}
$$

3 Application to Circumcoronene Series

Polycyclic aromatic hydrocarbons(PAH) are a class of organic compounds composed of aromatic rings. They may also have six-membered rings of various sizes that are not aromatic. Most of them are planar such as naphthalene, anthracene, and coronene. Sometimes, non-planarity is exhibited due to the topology of the molecule. Most of the PAHs have distinct physical and chemical properties, resulting in their significant contribution to material sciences and organic chemistry. Some of them are also being used in electronic devices. One such PAH which is grabbing most of the researchers' attention is coronene.

Coronene has a central arene unit completely enclosed by another outer ring of fused benzene rings C_6 in its circumference. The family generated in such a way from benzene rings is known as the circumcoronene series of Benzenoid H_k. The first few structures of this series are given in Figure 6. Various topological indices have been calculated for this series such as Zagreb indices, Szeged indices, Sanskruti index, eccentricity and connectivity indices, and many more. These can be accessed through the work cited here [2, 3, 7, 8, 9]. This paper focuses on the existing and newly formulated connection-based indices mentioned above. The molecular graph of a general circumcoronene series H_k is depicted in Figure 7. Using the edge-partition technique, we get the following cardinality of edges based on the possible ordered pairs of connection numbers 3, 4 & 6. Here, $k \geq 2$.

$$\begin{aligned}
\big|E_1\big| &= \big|\{uv \in E(H_k) \mid d_2(u) = 3, d_2(v) = 3\}\big| = 6,\\
\big|E_2\big| &= \big|\{uv \in E(H_k) \mid d_2(u) = 3, d_2(v) = 4\}\big| = 12,\\
\big|E_3\big| &= \big|\{uv \in E(H_k) \mid d_2(u) = 4, d_2(v) = 4\}\big| = 12(k-2),\\
\big|E_4\big| &= \big|\{uv \in E(H_k) \mid d_2(u) = 4, d_2(v) = 6\}\big| = 6(k-1),\\
\big|E_5\big| &= \big|\{uv \in E(H_k) \mid d_2(u) = 6, d_2(v) = 6\}\big| = 3(k-1)(3k-4).
\end{aligned}$$

The vertex-partition technique gives us the following vertex sets based on the connection numbers. Here, $k \geq 2$.

$$\begin{aligned}
\big|V_1\big| &= \big|\{u \in V(H_k) \mid d_2(u) = 3\}\big| = 12,\\
\big|V_2\big| &= \big|\{u \in V(H_k) \mid d_2(u) = 4\}\big| = 6(2k-3),\\
\big|V_3\big| &= \big|\{u \in V(H_k) \mid d_2(u) = 6\}\big| = 6(k-1)^2.
\end{aligned}$$

Theorem 3.1. *Let $H_k, k \geq 2$ be the chemical graph of the Circumcoronene series of benzenoid. Then*

$$\begin{aligned}
\text{(i)}FSO_L(H_k) &= \big[24\sqrt{97} + 108\sqrt{2}(3k-4)\big](k-1) + 192\sqrt{2}(k-2) +\\
&\quad 54\sqrt{2} + 12\sqrt{337},\\
\text{(ii)}^{m}FSO_L(H_k) &= \Big[\frac{3}{2\sqrt{97}} + \frac{3k-4}{12\sqrt{2}}\Big](k-1) + \frac{3(k-2)}{4\sqrt{2}} + \frac{2}{3\sqrt{2}} + \frac{12}{\sqrt{337}},\\
\text{(iii)}^{red}SO_L(H_k) &= \big[6\sqrt{34} + 15\sqrt{2}(3k-4)\big](k-1) + 36\sqrt{2}(k-2) +\\
&\quad 12(\sqrt{2} + \sqrt{13}),\\
\text{(iv)}^{2}FSO_L(H_k) &= \big[1990656 + 5038848(3k-4)\big](k-1) + 786432(k-2) +\\
&\quad 288198.
\end{aligned}$$

Proof. We get the following expressions for various connection-based indices using the defined edge sets.

(i) Using the definition of $FSO_L(G)$,

$$\begin{aligned}
FSO_L(H_k) = &\sum_{uv\in E_1}\sqrt{3^4+3^4}+\sum_{uv\in E_2}\sqrt{3^4+4^4}+\sum_{uv\in E_3}\sqrt{4^4+4^4}+\\
&\sum_{uv\in E_4}\sqrt{4^4+6^4}+\sum_{uv\in E_5}\sqrt{6^4+6^4}\\
=&6\times 9\sqrt{2}+12\sqrt{337}+12(k-2)\times 16\sqrt{2}+6(k-1)\times 4\sqrt{97}+\\
&3(k-1)(3k-4)\times 36\sqrt{2}\\
=&\big[24\sqrt{97}+108\sqrt{2}(3k-4)\big](k-1)+192\sqrt{2}(k-2)+54\sqrt{2}+\\
&12\sqrt{337}.
\end{aligned}$$

(ii) Using the definition of ${}^{m}FSO_L(G)$,

$$\begin{aligned}
{}^{m}FSO_L(H_k) = &\sum_{uv\in E_1}\frac{1}{\sqrt{3^4+3^4}}+\sum_{uv\in E_2}\frac{1}{\sqrt{3^4+4^4}}+\sum_{uv\in E_3}\frac{1}{\sqrt{4^4+4^4}}+\\
&\sum_{uv\in E_4}\frac{1}{\sqrt{4^4+6^4}}+\sum_{uv\in E_5}\frac{1}{\sqrt{6^4+6^4}}\\
=&\frac{6}{9\sqrt{2}}+\frac{12}{\sqrt{337}}+\frac{12(k-2)}{16\sqrt{2}}+\frac{6(k-1)}{4\sqrt{97}}+\frac{3(k-1)(3k-4)}{36\sqrt{2}}\\
=&\Big[\frac{3}{2\sqrt{97}}+\frac{3k-4}{12\sqrt{2}}\Big](k-1)+\frac{3(k-2)}{4\sqrt{2}}+\frac{2}{3\sqrt{2}}+\frac{12}{\sqrt{337}}.
\end{aligned}$$

(iii) From the definition of ${}^{red}SO_L(G)$,

$$\begin{aligned}
{}^{red}SO_L(H_k) = &\sum_{uv\in E_1}\sqrt{2^2+2^2}+\sum_{uv\in E_2}\sqrt{2^2+3^2}+\sum_{uv\in E_3}\sqrt{3^2+3^2}+\\
&\sum_{uv\in E_4}\sqrt{3^2+5^2}+\sum_{uv\in E_5}\sqrt{5^2+5^2}\\
=&6\times 2\sqrt{2}+12\sqrt{13}+12(k-2)\times 3\sqrt{2}+6(k-1)\sqrt{34}\\
&+[3(k-1)(3k-4)]\times 5\sqrt{2}\\
=&\big[6\sqrt{34}+15\sqrt{2}(3k-4)\big](k-1)+36\sqrt{2}(k-2)+12(\sqrt{2}+\sqrt{13}).
\end{aligned}$$

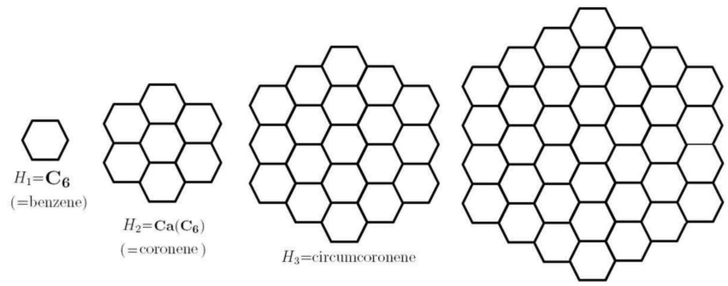


Figure 6: Chemical Graph of Some Members of Circumcoronene Series $H_k(k \geq 1)$ [2, 3, 4, 5, 7].

(iv) From the definition of ${}^2FSO_L(G)$,

$$\begin{aligned}
{}^2FSO_L(H_k) = & \sum_{uv \in E_1} 3^4 \times 3^4 + \sum_{uv \in E_2} 3^4 \times 4^4 + \sum_{uv \in E_3} 4^4 \times 4^4 + \\
& \sum_{uv \in E_4} 4^4 \times 6^4 + \sum_{uv \in E_5} 6^4 \times 6^4 \\
= & 39366 + 248832 + 12(k-2)65536 + 6(k-1)331776 \\
& + 3(k-1)(3k-4)1679616 \\
= & (k-1)\big[1990656 + 5038848(3k-4)\big] + 786432(k-2) + \\
& 288198. \quad \square
\end{aligned}$$

Theorem 3.2. *For the Circumcoronene series $H_k, k \geq 2$, we have*

(i) $SL(H_k) = \big[12\sqrt{13} + 18\sqrt{2}(3k-4)\big](k-1) + 48\sqrt{2}(k-2) + 18\sqrt{2} + 60,$

(ii) ${}^mSL(H_k) = \Big[\frac{3}{\sqrt{13}} + \frac{3k-4}{2\sqrt{2}}\Big](k-1) + \frac{3(k-2)}{\sqrt{2}} + \sqrt{2} + \frac{12}{5},$

(iii) $FL(H_k) = 1296(k-1)^2 + 384(2k-3) + 324,$

(iv) $F_1L(H_k) = \big[312 + 216(3k-4)\big](k-1) + 384(k-2) + 408.$

Proof. (i) Using the definition of $SL(G)$,

$$\begin{aligned}SL(H_k) = &\sum_{uv\in E_1}\sqrt{3^2+3^2}+\sum_{uv\in E_2}\sqrt{3^2+4^2}+\sum_{uv\in E_3}\sqrt{4^2+4^2}+\\&\sum_{uv\in E_4}\sqrt{4^2+6^2}+\sum_{uv\in E_5}\sqrt{6^2+6^2}\\=&6\times 3\sqrt{2}+12\times 5+12(k-2)\times 4\sqrt{2}+6(k-1)\times 2\sqrt{13}\\&+3(k-1)(3k-4)\times 6\sqrt{2}\\=&\big[12\sqrt{13}+18\sqrt{2}(3k-4)\big](k-1)+48\sqrt{2}(k-2)+18\sqrt{2}+60.\end{aligned}$$

(ii) Using the definition of ${}^mSL(G)$,

$$\begin{aligned}{}^mSL(H_k) = &\sum_{uv\in E_1}\frac{1}{\sqrt{3^2+3^2}}+\sum_{uv\in E_2}\frac{1}{\sqrt{3^2+4^2}}+\sum_{uv\in E_3}\frac{1}{\sqrt{4^2+4^2}}+\\&\sum_{uv\in E_4}\frac{1}{\sqrt{4^2+6^2}}+\sum_{uv\in E_5}\frac{1}{\sqrt{6^2+6^2}}\\=&\frac{6}{3\sqrt{2}}+\frac{12}{5}+\frac{12(k-2)}{4\sqrt{2}}+\frac{6(k-1)}{2\sqrt{13}}+\frac{3(k-1)(3k-4)}{6\sqrt{2}}\\=&\Big[\frac{3}{\sqrt{13}}+\frac{3k-4}{2\sqrt{2}}\Big](k-1)+\frac{3(k-2)}{\sqrt{2}}+\sqrt{2}+\frac{12}{5}.\end{aligned}$$

(iii) From the definition of $FL(G)$ and the vertex sets defined above,

$$\begin{aligned}FL(H_k) = &\sum_{u\in V_1}3^3+\sum_{u\in V_2}4^3+\sum_{u\in V_3}6^3\\=&12\times 27+6(2k-3)\times 64+6(k-1)^2\times 216\\=&1296(k-1)^2+384(2k-3)+324.\end{aligned}$$

(iv) From the definition of $F_1L(G)$,

$$\begin{aligned}F_1L(H_k) = &\sum_{uv\in E_1}3^2+3^2+\sum_{uv\in E_2}3^2+4^2+\sum_{uv\in E_3}4^2+4^2+\\&\sum_{uv\in E_4}4^2+6^2+\sum_{uv\in E_5}6^2+6^2\\=&408+12(k-2)32+6(k-1)52+3(k-1)(3k-4)72\\=&(k-1)\big[312+216(3k-4)\big]+384(k-2)+408.\quad\square\end{aligned}$$

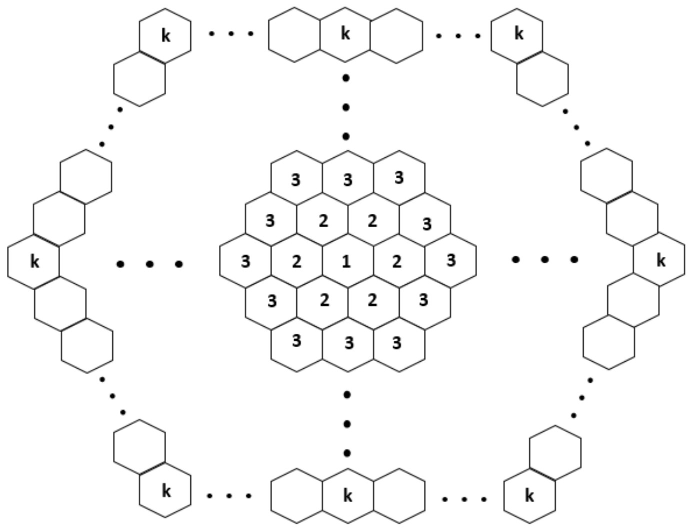
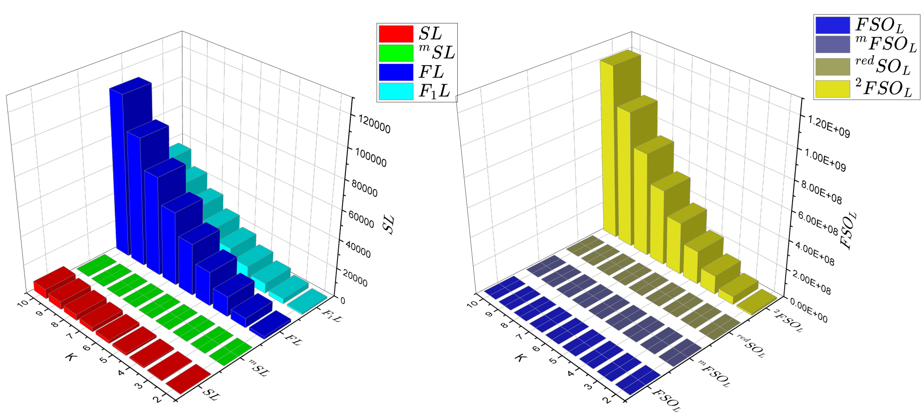


Figure 7: Chemical Graph of Circumcoronene Series of Benzenoid $H_k (k \geq 1)$.



(a) **(b)**

Figure 8: Characteristic Trend of $H_K (k \geq 2)$.

Table 1: Values of Connection Indices for Circumcoronene Series of Benzenoid $H_K(k \geq 2)$.

k	SL	^{m}SL	FL	F_1L	FSO_L	$^{m}FSO_L$	$^{red}SO_L$	$^{2}FSO_L$
2	179.6341	5.3534	2004	1152	838.501	1.3952	137.6493	12356550
3	494.4297	11.1351	6660	3576	2568.2830	2.5492	393.2523	55444422
4	928.0193	17.9776	13908	7104	5078.7110	3.7917	750.6787	128372166
5	1514.3439	26.9414	23748	11928	8505.5494	5.3876	1235.3843	231532998
6	2253.4036	38.0265	36180	18048	12848.7982	7.3372	1847.3691	364926918
7	3145.1983	51.2329	51204	25464	18108.4574	9.6403	2586.6332	528553926
8	4189.7282	66.5606	68820	34176	24284.5269	12.2969	3453.1765	722414022
9	5386.9930	84.0097	89028	44184	31377.0068	15.3071	4446.9990	946507206
10	6736.9930	103.5801	111828	55488	39385.8972	18.6708	5568.1007	1200833478

3.1 Graphical analysis

Table 1 represents the values of all the above eight leap indices calculated for the Circumcoronene series of Benenoid $H_k, k \geq 2$ using Theorems 3.1 and 3.2. The graphs are plotted for all the indices against k-values using these values, which are depicted in Figure 8. From Figure 8a, it can be noticed that the FL has shown a rapid increase in its values with an increase in the 'k' value. In Figure 8b, $^{2}FSO_L$ has shown a similar trend. But, $^{2}FSO_L$ has proved its high discriminative power in terms of its values for the Circumcoronene series with different 'k' values compared to FL. Hence, it can be concluded that the second F-Sombor leap index $^{2}FSO_L$, formulated by the authors, can be used for the characteristic and topological study of the Circumcoronene series of Benzenoid H_k.

4 Conclusion

The mathematical closed-form expressions of various leap indices have been formulated for path, cycle, and special graphs like wheel, windmill, and friendship graphs with the single edge-partition technique. These exact expressions can be directly applied to molecules, structures, and networks whose chemical graphs are similar to the above graphs. We have also formulated the closed-form expressions for a Circumcoronene series of Benzenoid and depicted them in a graph showing the structure's characteristic trend. Similarly, the exact expressions of unexplored topological indices for various graphs and structures can be formulated.

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