Research Article

Valency-Based Topological Properties of Linear Hexagonal Chain and Hammer-Like Benzenoid

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Received 8 March 2021; Revised 26 March 2021; Accepted 11 April 2021; Published 27 April 2021

Academic Editor: Huihua Chen

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Topological indices are quantitative measurements that describe a molecule’s topology and are quantified from the molecule’s graphical representation. The significance of topological indices is linked to their use in QSPR/QSAR modelling as descriptors. Mathematical associations between a particular molecular or biological activity and one or several biochemical and/or molecular structural features are QSPRs (quantitative structure-property relationships) and QSARs (quantitative structure-activity relationships). In this paper, we give explicit expressions of two recently defined novel ev-degree- and ve-degree-based topological indices of two classes of benzenoid, namely, linear hexagonal chain and hammer-like benzenoid.

1. Introduction

The combination of graph theory and chemistry is called chemical graph theory. An important use of graph theory is to mathematically model molecules. This helps the researchers to gain insight into the physical properties of these chemical compounds. Some physical properties such as the boiling point are related to the geometric structure of the compound. The chemical compounds have a variety of applications in pharmaceutical chemistry. In chemistry, numerous compounds of different structures have the same chemical formula [1]. The chemical graph theory is a fast-rising field among researchers with applications in chemistry, biological, and electrical networks and drug designs [2–5].

In the QSPR/QSAR analyses, scientists are interested in studying the topology of chemical networks linked to medicine, drug design, medical research, and experimental science using certain mathematical parameters obtained from the molecular structures of these networks [6]. Different properties or behaviors of chemical molecules have been investigated in the field of quantitative structure-property relationships [7, 8].

Benzene is colorless and odour characteristic aromatic compound. Michael Faraday first isolated and identified benzene [9, 10]. Then, Eilhard Mitscherlich produced it by lime and benzoic acid [11], and Charles Mansfield from coal tar [12]. August Kekulé proposed the ring structure of six carbon atoms [13]. A big amount of benzene is used to manufacture cumene for phenol, and other amount is used in the manufacture of nylon fibers, detergents, drugs, and pesticides. Benzene is mobilized in the human body because of its exposure from tobacco smoke exhaust from motor vehicles and industries [14]. The compound having only benzene rings is known as the benzenoid aromatic compound.

The topological descriptor concept was firstly given by Wiener [15] when working on paraffin, and the index number is correlated with the critical point, boiling points, and density [16, 17]. The topological indices are used to understand and develop mathematical characteristics of models by using edge, vertex, and degree concept. Mostly Randic, Wiener, and
Zagreb indices are used in chemical and mathematical literature [18–21]. The Randić index variant is the harmonic index defined by Zhong [22]. However, all of the above research was performed by utilizing the classical concept of degrees. Chellali et al. introduced ve-degree and ev-degree [23], and Horoldagva et al. explored Chellali et al.’s work and gave mathematical concepts [24]. The degree-based ideology transformed into ve-degree and ev-degree.

In this paper, we have discussed few ideologies of ve-degree and ev-degree. We present the ve-degree- and ev-degree-based topological indices for the molecular structure of multiple segment linear hexagonal chain $L[m,n]$ and hammer like benzenoid $H_m$. We have presented ve-degree- and ev-degree-based topological indices for the molecular structure of for molecular structure of multiple segment linear hexagonal chains $L[m,n]$ and hammer-like benzenoid $H_m$. There is a wide-ranging research activity now on ve-degree- and ev-degree-based topological indices or variants. For further explanation of these topological indexes of different graphs and chemical structures, see [25–38].

Let $G$ be a graph with vertex set $V(G)$ and edge set $E(G)$. For any vertex $v \in V(G)$, let $\delta(v)$ denotes the degree of $v$ and is defined as the number of edges incident to $v$. The open neighborhood of $v$ is denoted by $N(v)$ and is defined as the set of vertices adjacent to $v$. The closed neighborhood of $v$, denoted by $N[v]$ is defined as $N[v] = N(v) \cup v$.

The ev-degree of any edge $uv = e \in E(G)$ is the total number of the vertices of closed neighborhoods of the end vertices of an edge $e$, and the ev degree is denoted by $\Lambda_{ve}(e)$.

The ve-degree of any vertex $v \in V(G)$ is the total number of different edges which is adjacent to $v$ and the first neighbors of $v$, i.e., the sum of degrees of all closed neighborhood vertices of $v$.

### 2. Ev-Degree-Based Indices

For a connected graph $G$, the ev-degree-based Zagreb ($M^e$) index and Randic ($R^e$) index for any edge $e = uv \in E(G)$ are defined as

\[
M^e_e(G) = \sum_{e \in E} \Lambda_{ve}(e)^2, \\
R^e_e(G) = \sum_{e \in E} \Lambda_{ve}(e)^{-1/2}. 
\]

2.1. Ve-Degree-Based Index. For a connected graph $G$, the ve-degree-based first Zagreb alpha ($M^{ve}_1$) index for any vertex $v \in V(G)$ is defined as

\[
M^{ve}_1(G) = \sum_{v \in V} \Lambda_{ve}(v)^2. 
\]

2.2. End Vertices’ Ve-Degree-Based Indices of Each Edge. For a connected graph $G$, the end vertices’ ve-degree-based indices for each edge, such as ve-degree-based first Zagreb beta index ($M^{ve}_1$), second Zagreb beta index ($M^{ve}_2$), atom-bond connectivity index (ABC$^e$) [18], geometric-arithmetic index (GA$^e$) [39], harmonic index (H$^e$), sum-connectivity index ($\chi$) [40], and the Randic index ($R^{ve}$) for each edge $uv \in E(G)$, are defined as

\[
M^{ve}_1(G) = \sum_{uv \in E} (\Lambda_{ve}(u) + \Lambda_{ve}(v)), \\
M^{ve}_2(G) = \sum_{uv \in E} (\Lambda_{ve}(u) \times \Lambda_{ve}(v)), \\
ABC^{ve}(G) = \sum_{uv \in E} \left( \frac{\Lambda_{ve}(u) + \Lambda_{ve}(v) - 2}{\Lambda_{ve}(u) \times \Lambda_{ve}(v)} \right), \\
GA^{ve}(G) = \sum_{uv \in E} \frac{2\Lambda_{ve}(u) \times \Lambda_{ve}(v)}{\Lambda_{ve}(u) + \Lambda_{ve}(v)}, \\
H^{ve}(G) = \sum_{uv \in E} \frac{2}{\Lambda_{ve}(u) + \Lambda_{ve}(v)}, \\
\chi^{ve}(G) = \sum_{uv \in E} (\Lambda_{ve}(u) + \Lambda_{ve}(v))^{-1/2}, \\
R^{ve}(G) = \sum_{uv \in E} (\Lambda_{ve}(u) \times \Lambda_{ve}(v))^{-1/2}. 
\]

### 3. Benzenoid

Benzene is an important parent aromatic compound of highly toxic nature having colorless and odour characteristics. Benzene is widely used in production volume such as to make synthetic fibers, dyes, plastic, resins, polystyrene, drugs, and pesticides and ranks in the top 20 chemicals [41]. The biggest application of benzene is in phenol preparation. Soon after its industrial use began, the toxicity of benzene was noticed in the blood forming organs [41]. In 1897, nine cases of benzene hematotoxicity were described [42] and further effects were documented in Weiskotten [43, 44] and Selliing [45]. In 1928, the first case of benzene-related leukemia in a man was reported [41]. Benzene was first obtained from coal tar which was then replaced by processes based on petroleum. Chemist considered benzene puzzling in the 19th century that it could be so unreactive against additional reactions, considering its high degree of unsaturation. In 1865, finally, Kekulé proposed the ring structure [13]. We use commonly six carbon atoms that form a ring with an alternative single and double bond. The aromatic compound having only benzene rings in its form is known as the benzenoid aromatic compound. The multiple segment linear hexagonal chain of benzenoid is a prominent family of molecular benzenoid graphs, where this family formed on segment solely from benzenoid C6 (hexagon).

3.1. Crystallographic Structure of Multiple Segment Linear Hexagonal Chain $L[m,n]$. In this paper, we discuss two classes of benzenoid system, and first is a multiple segment linear hexagonal chains. A finite connected subgraph of the
infinite hexagonal lattice without cut vertices or non-hexagonal interior faces is said to be a benzenoid system. In multiple segment linear hexagonal chains, six carbon atoms are connected through bond with angle 120° form hexagonal structure. Benzenoid system is called peri-condensed if three hexagons are connected by common vertex; otherwise, we say catacondensed.

The acenes or polyacenes are a class of organic compounds and polycyclic aromatic hydrocarbons made up of linearly fused benzene rings. A linear chain of finite hexagonal structure rings of finite segments is called multiple segment linear hexagonal chains $L[m, n]$. From Figure 1, we can obtain a single armchair chain for $m = 2$ and $n \geq 2$. The crystal structure of $L[m, n]$ contains the $2(4mn - 4n + 3)$ vertices and $2(5mn - 5n + 3)$ edges, where $m \geq 2$ and $n \geq 2$. On the basis of degree of vertices, we divide it into two partitions in such way: $2(2mn - 2n + 3)$ vertices of degree 2 and $4mn - 4n$ vertices of degree 3. Similarly, the edges of $L[m, n]$ are partitioned as $E_{(2,2)}$ with $2n + 5$ edges, $E_{(2,3)}$ with $8mn - 12n + 2$ edges, and $E_{(3,3)}$ having $2mn - 1$ edges.

4. Main Results

Theorem 1. Let $H$ be a molecular graph of multiple segment linear hexagonal chains $L[m, n]$; then, ev-degree-based Zagreb index and ev-degree-based Randic index are given by

(i) $\mathcal{M}^e(H) = 272mn - 268n + 94.$

(ii) $\mathcal{R}^e(H) = (8/\sqrt{5} + 2/\sqrt{6})mn + (1 - 12/\sqrt{5})n + (5/2 + 2/\sqrt{5} - 1/\sqrt{6}).$

Proof. From the structure of multiple segment linear hexagonal chain $L[m,n]$, there are three types of the edge partitions $E_{(2,2)}$, $E_{(2,3)}$, and $E_{(3,3)}$ respectively, where the total number of the edges is $2(5mn - 5n + 3)$. By the definition of ev-degree, we have calculated the ev-degrees of the given edges partition as shown in Table 1. From Table 1, we have proved ev-degree-based indices such as

(i) The ev-degree-based Zagreb index:

\[ \mathcal{M}^e(H) = \sum_{e \in E(H)} A_v(e) \]

\[ \mathcal{M}^e(H) = (4)^2 |E_{(2,2)}| + (5)^2 |E_{(2,3)}| + (6)^2 |E_{(3,3)}| \]

\[ = (4)^2 (2n + 5) + (5)^2 (8mn - 12n + 2) + (6)^2 (2mn - 1) \]

\[ = (16)(2n + 5) + (25)(8mn - 12n + 2) + (36)(2mn - 1) \]

\[ = 272mn - 268n + 94. \] (4)

(ii) The ev-degree-based Randic index:

\[ \mathcal{R}^e(H) = \sum_{e \in E(H)} \Lambda_{ev}(e)^{-(1/2)}, \]

\[ \mathcal{R}^e(H) = (4)^{-1/2}|E_{(2,2)}| + (5)^{-1/2}|E_{(2,3)}| + (6)^{-1/2}|E_{(3,3)}| \]

\[ = (4)^{-1/2}(2n + 5) + (5)^{-1/2}(8mn - 12n + 2) \]

\[ + (6)^{-1/2}(2mn - 1) \]

\[ = \left( \frac{8}{\sqrt{5}} + \frac{2}{\sqrt{6}} \right)mn + \left( 1 - \frac{12}{\sqrt{5}} \right)n + \left( \frac{5}{2} + \frac{2}{\sqrt{5}} - \frac{1}{\sqrt{6}} \right). \] (5)

Theorem 2. Let $H$ be a molecular graph of segment linear hexagonal chain $L[m, n]$; then, vertices’ ve-degree-based first Zagreb a-index is given by

\[ \mathcal{N}_1^{ev} (H) = 340mn - 324n + 84. \] (6)

Proof. From the structure of linear hexagonal chain $L[m,n]$, we divide the vertices into two partitions on the basis of degrees $V_2$ and $V_3$, respectively, where the total number of the vertices is $2(4mn - 4n + 3)$. By the definition of ve-degrees, we have calculated the vertices’ ve-degrees as shown in Table 2.

By using above table, we have first ve-degree-based Zagreb a-index.

\[ \mathcal{N}_1^{ev} (H) = \sum_{v \in V(H)} A_v(v)^2 \]

\[ \mathcal{N}_1^{ev} (H) = (4)^2 (4) + (5)^2 (4n + 2) + (6)^2 (4mn - 8n) \]

\[ + (7)^2 (4nn - 8n + 2) + (8)^2 (4n - 2) \]

\[ = 340mn - 324n + 84. \]

Theorem 3. Let $H$ be a molecular graph of linear hexagonal chain $L[m, n]$; then, end vertices’ ve-degree-based indices of each edges are given by

(i) $\mathcal{N}_1^{ev} (H) = 134nn - 134n + 48$

(ii) $\mathcal{N}_2^{ev} (H) = 448nn - 442n + 81$

(iii) ABC$^e(H) = (8\sqrt{11}/\sqrt{42} + 2\sqrt{13}/\sqrt{56})mn +$

\[ (2\sqrt{8}/5 + 4\sqrt{2}/\sqrt{7} - 20\sqrt{11}/\sqrt{42} + 2 - 2\sqrt{13}/\sqrt{56} + \]

\[ \sqrt{14}/4)n + (\sqrt{6}/2 + 2\sqrt{7}/\sqrt{5} - \sqrt{8}/5 + 2\sqrt{2}/\sqrt{7} + \]

\[ 2\sqrt{11}/\sqrt{42} - \sqrt{14}/8 - 1) \]

(iv) GA$^e(H) = (16\sqrt{42}/13 + 4\sqrt{56}/15)mn +$

\[ (2\sqrt{35}/3 + \]

\]
there are three types of edge partitions based indices of each edge such as \((\Lambda(u), \Lambda(v))\), \(\Lambda_{ev}(e)\), and \(\Lambda_{ve}(v)\), respectively, where the total number of the edges is \(2(5mn - 5n + 3)\). According to definition of ve-degree of end vertices of each edge, we divide the new edges into five partitions, i.e., \(E_1^v\), \(E_2^v\), \(E_3^v\), \(E_4^v\), \(E_5^v\), \(E_6^v\), \(E_7^v\), and \(E_8^v\), respectively, as shown in Table 3.

By using the table, we can prove end vertices’ ve-degree-based indices of each edge such as

(i) The first Zagreb \(\beta\)-index:

\[
W_1^{\beta}(H) = \sum_{u \in E(H)} (\Lambda_{ve}(u) + \Lambda_{ve}(v)),
\]

\[
E_1^{\beta}(H) = \sum_{u \in E(H)} (\Lambda_{ve}(u) + \Lambda_{ve}(v)),
\]

\[
E_2^{\beta}(H) = (8) |E_1^v| + (9) |E_2^v| + (10) |E_3^v|
\]

\[
+ (12) |E_4^v| + (13) |E_5^v| + (14) |E_6^v|
\]

\[
+ (15) |E_7^v| + (16) |E_8^v|
\]

\[
= (8)(2) + (9)(4) + (10)(2n - 1)
\]

\[
+ (12)(4n + 2) + (13)(8mn - 20n + 2)
\]

\[
+ (14)(4n - 2) + (15)(2mn - 2n)
\]

\[
+ (16)(2n - 1)
\]

\[
= 134mn - 134n + 48.
\]

(ii) The second Zagreb beta index:

\[
W_2^{\beta}(H) = \sum_{u \in E(H)} (\Lambda_{ve}(u)\Lambda_{ve}(v)),
\]

\[
E_1^{\beta}(H) = (16) |E_1^v| + (20) |E_2^v| + (25) |E_3^v|
\]

\[
+ (35) |E_4^v| + (42) |E_5^v| + (48) |E_6^v|
\]

\[
+ (56) |E_7^v| + (64) |E_8^v|
\]

\[
= (16)(2) + (20)(4) + (25)(2n - 1)
\]

\[
+ (35)(4n + 2) + (42)(8mn - 20n + 2)
\]

\[
+ (48)(4n - 2) + (56)(2mn - 2n)
\]

\[
+ (64)(2n - 1)
\]

\[
= 448mn - 442n + 81.
\]

(iii) The atom-bond connectivity index:
Table 3: End vertices' ve-degrees of each edge of $L[m, n]$.

| Edge $E_i$ | $(\lambda_{ve}(u), \lambda_{ve}(v))$ | Frequency |
|------------|---------------------------------|-----------|
| $E_1$     | (4, 4)                          | 2         |
| $E_2$     | (4, 5)                          | 4         |
| $E_3$     | (5, 5)                          | $2n - 1$  |
| $E_4$     | (5, 7)                          | $4n + 2$  |
| $E_5$     | (6, 7)                          | $4n + 2$  |
| $E_6$     | (5, 7)                          | $4n + 2$  |
| $E_7$     | (7, 8)                          | $2mn - 2n$|
| $E_8$     | (8, 8)                          | $2n - 1$  |

$$ \text{ABC}^v(H) = \sum_{u \in V(H)} \left[ \sqrt{\lambda_{ve}(u) + \lambda_{ve}(v) - 2} \right] \mathcal{G}^v(H) = \sum_{u \in V(H)} \frac{2\sqrt{\lambda_{ve}(u) \times \lambda_{ve}(v)}}{\lambda_{ve}(u) + \lambda_{ve}(v)}$$

$$ \text{ABC}^v(H) = \left( \frac{6}{16} \right) |E_1| + \left( \frac{7}{20} \right) |E_2| + \left( \frac{8}{25} \right) |E_3|$$

$$ + \left( \frac{10}{35} \right) |E_4| + \left( \frac{11}{42} \right) |E_5|$$

$$ + \left( \frac{12}{48} \right) |E_6| + \left( \frac{13}{56} \right) |E_7| + \left( \frac{14}{64} \right) |E_8|$$

$$= \left( \frac{6}{16} \right) (2) + \left( \frac{7}{20} \right) (4) + \left( \frac{8}{25} \right) (2n - 1)$$

$$+ \left( \frac{10}{35} \right) (4n + 2) + \left( \frac{11}{42} \right)$$

$$\times (8mn - 20 + 2) + \left( \frac{12}{48} \right) (4n - 2)$$

$$+ \left( \frac{13}{56} \right) (2mn - 2n) + \left( \frac{14}{64} \right) (2n - 1)$$

$$= \frac{8\sqrt{11}}{\sqrt{42}} + \frac{2\sqrt{13}}{\sqrt{56}} mn$$

$$+ \left( \frac{2\sqrt{8}}{5} + \frac{4\sqrt{2}}{\sqrt{7}} + \frac{20\sqrt{11}}{\sqrt{42}} - 2 \frac{2\sqrt{13}}{\sqrt{56}} + \frac{\sqrt{14}}{4} \right)n$$

$$+ \left( \frac{\sqrt{5}}{2} + \frac{2\sqrt{\gamma}}{\sqrt{5}} - \frac{\sqrt{2}}{\sqrt{5}} + \frac{4\sqrt{2}}{\sqrt{42}} \frac{\sqrt{14}}{8} - 1 \right).$$

(10)

(iv) The geometric-arithmetic index:

(v) The harmonic index:
\( \chi^{\star}(H) = \sum_{u \in V(H)} (\Lambda_{uv}(u) + \Lambda_{uv}(v))^{-1/2}, \)

\( \chi^{\star}(H) = (8)^{-1/2} |E| + (9)^{-1/2} |E_2| + (10)^{-1/2} |E_3| \\
+ (12)^{-1/2} |E_4| + (13)^{-1/2} |E_5| + (14)^{-1/2} |E_6| \\
+ (15)^{-1/2} |E_7| + (16)^{-1/2} |E_8| \\
= (8)^{-1/2} (2) + (9)^{-1/2} (4) + (10)^{-1/2} (2n - 1) \\
+ (12)^{-1/2} (4n + 2) + (13)^{-1/2} (8mn - 20n + 2) \\
+ (14)^{-1/2} (4n - 2) + (15)^{-1/2} (2mn - 2n) \\
+ (16)^{-1/2} (2n - 1) \\
= \left(\frac{8}{\sqrt{13}} + \frac{2}{\sqrt{15}}\right)^{mn} \\
\times \left(\frac{2}{\sqrt{10}} + \frac{2}{\sqrt{13}} + \frac{20}{\sqrt{13}} + \frac{4}{\sqrt{14}} - \frac{2}{\sqrt{15}} + \frac{1}{2}\right)^{n} \\
\times \left(\frac{2}{\sqrt{8}} + \frac{4}{\sqrt{9}} - \frac{1}{\sqrt{10}} + \frac{2}{\sqrt{12}} + \frac{2}{\sqrt{13}} - \frac{2}{\sqrt{14}} - \frac{1}{4}\right). \) (13)

(vii) The Randic index:

\[ R^{\star}(H) = \sum_{uv \in E(H)} (\Lambda_{uv}(u)\Lambda_{uv}(v))^{-(1/2)}. \]

\[ R^{\star}(H) = (16)^{-1/2} |E| + (20)^{-1/2} |E_2| \\
+ (25)^{-1/2} |E_3| + (35)^{-1/2} |E_4| + (42)^{-1/2} |E_5| \\
+ (48)^{-1/2} |E_6| + (56)^{-1/2} |E_7| + (64)^{-1/2} |E_8| \\
= (16)^{-1/2} (2) + (20)^{-1/2} (4) + (25)^{-1/2} (2n - 1) \\
+ (35)^{-1/2} (4n + 2) + (42)^{-1/2} (8mn - 20n + 2) \\
+ (48)^{-1/2} (4n - 2) + (56)^{-1/2} (2mn - 2n) \\
+ (64)^{-1/2} (2n - 1) \\
= \left(\frac{8}{\sqrt{42}} + \frac{1}{\sqrt{14}}\right)^{mn} \\
\times \left(\frac{2}{5} + \frac{4}{\sqrt{35}} + \frac{20}{\sqrt{42}} + \frac{1}{\sqrt{13}} - \frac{1}{\sqrt{14}} + \frac{1}{4}\right)^{n} \\
\times \left(\frac{7}{\sqrt{40}} + \frac{2}{\sqrt{5}} + \frac{2}{\sqrt{35}} + \frac{2}{\sqrt{42}} - \frac{1}{2\sqrt{3}}\right). \) (14)

4.1. Crystallographic Structure of Hammer-Like Benzenoid \( H_n \). Now, we discuss the second class of the benzenoid system that is a hammer-like structure. The linear polyacene of length \( n \) and both ends of polyacene are connected by pyrene fragments. Benzenoid system is called peri-condensed if three hexagons are connected by common vertex; otherwise, we say catacondensed. \( H_n \) is not a catacondensed benzenoid because a peri-condensed group is connected at end of polyacene, but in this paper, we discuss the structure of \( H_n \) as the varying fragments are catacondensed [46].

We can obtain the hammer-like benzene structure \( H_n \) by terminating the ends of a linear polyacene of length \( n \) with two pyrene fragments (see Figure 2). The crystal structure of \( H_n \) contains the \( 2(2n + 15) \) vertices and \( 5n + 39 \) edges. On the basis of degree of vertices, we divide it into two partitions in such way: \( 2(n + 8) \) vertices of degree 2 and \( 2(n + 7) \) vertices of degree 3. Similarly, the edges of \( H_n \) are partitioned as \( E_{(2,2)} \) with 10 edges, \( E_{(2,3)} \) with \( 4n + 12 \) edges, and \( E_{(3,3)} \) having \( n + 15 \) edges.

5. Main Results

Theorem 4. Let \( H \) be a molecular graph of hammer-like structure \( H_n \), then, ev-degree-based Zagreb index and ev-degree-based Randic index are given by
(i) $M_{ev}^{t}(H) = 136n + 1000.$
(ii) $R_{ev}^{t}(H) = (4/\sqrt{5} + 1/\sqrt{6})n + (12/\sqrt{5} + 15/\sqrt{6} + 5)$.

**Proof.** From the structure of hammer-like structure $H_n$, there are three types of the edge partitions $E_{(2,2)}$, $E_{(2,3)}$, and $E_{(3,3)}$, respectively, where the total number of the edges is $5n + 39$. By the definition of ev-degree, we have calculated the ev-degrees of the given edges partition as shown in Table 4.

From Table 4, we have proved ev-degree-based indices such as

(i) The ev-degree-based Zagreb index:

$$M_{ev}^{t}(H) = \sum_{e \in E(H)} \Lambda_{ev}(e)^2,$$

$$M_{ev}^{t}(H) = (4^2|E_{(2,2)}| + (5)^2|E_{(2,3)}| + (6)^2|E_{(3,3)}|)$$

$$= (4^2(10) + (5)^2(4n + 12) + (6)^2(n + 15))$$

$$= (16)(10) + (25)(4n + 12) + (36)(n + 15)$$

$$= 136n + 1000.$$  \hspace{1cm} (15)

(ii) The ev-degree-based Randic index:

$$R_{ev}^{t}(H) = \sum_{e \in E(H)} \Lambda_{ev}(e)^{-1/2},$$

$$R_{ev}^{t}(H) = (4)^{-1/2}|E_{(2,2)}| + (5)^{-1/2}|E_{(2,3)}| + (6)^{-1/2}|E_{(3,3)}|$$

$$= (4)^{-1/2}(10) + (5)^{-1/2}(4n + 12) + (6)^{-1/2}(n + 15)$$

$$= \left(\frac{4}{\sqrt{5}} + \frac{1}{\sqrt{6}}\right)n + \left(\frac{12}{\sqrt{5}} + \frac{15}{\sqrt{6}} + 5\right).$$  \hspace{1cm} (16)

**Theorem 5.** Let $H$ be a molecular graph of hammer-like structure $H_n$; then, vertices’ ve-degree-based first Zagreb $\alpha$-index is given by

$$M_{1}^{ve}(H) = 170n + 1298.$$  \hspace{1cm} (17)

**Proof.** From the structure of hammer-like structure $H_n$, we divide the vertices into two partitions on the basis of degrees $V_2$ and $V_3$, respectively, where the total number of the vertices is $2(2n + 15)$. By the definition of ve-degrees, we have calculated the vertices’ ve-degrees as shown in Table 5.

By using Table 5, we have first ve-degree-based Zagreb $\alpha$-index:

$$M_{1}^{ve}(H) = \sum_{v \in V(H)} \Lambda_{ve}(v)^2,$$

$$M_{1}^{ve}(H) = (4)^2(4) + (5)^2(12) + (6)^2(2n) + (7)^2(2n + 2) + (8)^2(8) + (9)^2(4)$$

$$= 170n + 1298.$$  \hspace{1cm} (18)

**Theorem 6.** Let $H$ be a molecular graph of hammer-like structure $H_n$; then, end vertices’ ve-degree-based indices of each edge are given by

(i) $M_{1}^{ve}(H) = 66n + 494$
(ii) $M_{1}^{ve}(H) = 217n + 1711$
(iii) $ABC_{ev}(H) = (4\sqrt{11}/\sqrt{42} + \sqrt{12}/7)n + (8\sqrt{7}/\sqrt{20} + 4\sqrt{1/5} + 8/\sqrt{3} + 4\sqrt{11}/\sqrt{42} + 4\sqrt{5}/\sqrt{34} + 3\sqrt{14}/4 + 8/9 - 4\sqrt{11}/\sqrt{42} - \sqrt{12}/7 + 4\sqrt{14}/\sqrt{63} + 2)$
Proof. From the structure of hammer-like structure $H_n$, there are three types of edge partitions $E_{(2,2)}$, $E_{(2,3)}$, and $E_{(3,3)}$, respectively, where the total number of the edges is $5n + 39$. According to definition of ve-degree of end vertices of each edge, we divide the new edges into eleven partitions, i.e., $E'_1$, $E''_1$, $E'_2$, $E''_2$, $E'_3$, $E''_3$, $E'_4$, $E''_4$, $E'_5$, $E''_5$, $E'_6$, $E''_6$, $E'_{10}$, and $E'_{11}$, respectively, as shown in Table 6.

By using the Table 6, we can prove end vertices’ ve-degree-based indices of each edge such as

(i) The first Zagreb $\beta$-index:

$$M^\beta_1 (H) = \sum_{uv \in E(H)} (\Lambda_{ve}(u) + \Lambda_{ve}(v)),$$

(ii) The second Zagreb beta-index:

$$M^\beta_2 (H) = \sum_{uv \in E(H)} (\Lambda_{ve}(u)\Lambda_{ve}(v)).$$

(iii) The atom-bond connectivity index:

$$\frac{\sqrt{2}}{\sqrt{17} + 9} (iv) \, GA^w (H) = (8\sqrt{42}/13 + 1)n + (16\sqrt{20}/9 + 4\sqrt{35}/3 + 8\sqrt{40}/13 + 16\sqrt{3}/7 + 8\sqrt{42}/13 + 6\sqrt{7}/4 + 24\sqrt{2}/17 + 9)$$

(v) $R^w (H) = 69/91n + 42001/7140$

(vi) $\chi^w (H) = (4/\sqrt[4]{13} + 1/\sqrt[4]{14})n + (8/9 + 2/10 + 8/\sqrt[4]{12} + 3/2 + 4/\sqrt[4]{17} + 2/17 + 1)$

(vii) $\Lambda^w (H) = (4/\sqrt[4]{42} + 1/7)n + (4/\sqrt[4]{5} + 2/5 + 8/\sqrt[4]{35} + 2/\sqrt[4]{10} + 1/\sqrt[4]{3} + 4/\sqrt[4]{42} + 1/7 + 4/\sqrt[4]{7} + 2/3/2 + 3/4 + 2/9)$

Table 5: The vertices’ ve-degrees of $H_n$.  

| $\Lambda (u)$ | $\Lambda_{ve} (u)$ | Frequency |
|--------------|------------------|-----------|
| 2            | 4                |           |
| 2            | 5                | 12        |
| 3            | 6                | 2n        |
| 3            | 7                | 2n + 2    |
| 3            | 8                | 8         |
| 3            | 9                | 4         |

Table 6: End vertices’ ve-degrees of each edge of $H_n$.  

| Edge        | $\Lambda_{ve} (u) \Lambda_{ve} (v)$ | Frequency |
|-------------|-------------------------------------|-----------|
| $E'_1$      | (4, 5)                              | 8         |
| $E'_2$      | (5, 5)                              | 2         |
| $E'_3$      | (5, 7)                              | 8         |
| $E'_4$      | (5, 8)                              | 4         |
| $E'_5$      | (6, 7)                              | 4n - 4    |
| $E'_6$      | (6, 8)                              | 4         |
| $E'_7$      | (7, 7)                              | n - 1     |
| $E'_8$      | (7, 9)                              | 4         |
| $E'_9$      | (8, 8)                              | 6         |
| $E'_{10}$   | (8, 9)                              | 4         |
| $E'_{11}$   | (9, 9)                              | 2         |

$\sqrt{17}$
The geometric-arithmetic index:

\[
\text{GA}^{\text{ve}}(H) = \sum_{uv \in E(H)} \frac{2\sqrt{\Lambda_{\text{ve}}(u) \times \Lambda_{\text{ve}}(v)}}{\Lambda_{\text{ve}}(u) + \Lambda_{\text{ve}}(v)},
\]

\[
\text{GA}^{\text{ve}}(H) = \left( \frac{2\sqrt{\frac{20}{9}}}{9} \right) |E^*_1| + \left( \frac{2\sqrt{\frac{25}{10}}}{10} \right) |E^*_2| + \left( \frac{2\sqrt{\frac{35}{12}}}{12} \right) |E^*_3| + \left( \frac{2\sqrt{\frac{40}{13}}}{13} \right) |E^*_4| + \left( \frac{2\sqrt{\frac{42}{13}}}{13} \right) |E^*_5|
\]

\[
+ \left( \frac{2\sqrt{\frac{48}{14}}}{14} \right) |E^*_6| + \left( \frac{2\sqrt{\frac{49}{14}}}{14} \right) |E^*_7| + \left( \frac{2\sqrt{\frac{63}{16}}}{16} \right) |E^*_8| + \left( \frac{2\sqrt{\frac{64}{16}}}{16} \right) |E^*_9|
\]

\[
+ \left( \frac{2\sqrt{\frac{72}{17}}}{17} \right) |E^*_10| + \left( \frac{2\sqrt{\frac{81}{18}}}{18} \right) |E^*_11|
\]

\[
= \left( \frac{2\sqrt{\frac{20}{9}}}{9} \right) (8) + \left( \frac{2\sqrt{\frac{25}{10}}}{10} \right) (2) + \left( \frac{2\sqrt{\frac{35}{12}}}{12} \right) (8) + \left( \frac{2\sqrt{\frac{40}{13}}}{13} \right) (4) + \left( \frac{2\sqrt{\frac{42}{13}}}{13} \right) (4n - 4)
\]

\[
+ \left( \frac{2\sqrt{\frac{48}{14}}}{14} \right) (4) + \left( \frac{2\sqrt{\frac{49}{14}}}{14} \right) (n - 1) + \left( \frac{2\sqrt{\frac{63}{16}}}{16} \right) (4) + \left( \frac{2\sqrt{\frac{64}{16}}}{16} \right) (6)
\]

\[
+ \left( \frac{2\sqrt{\frac{72}{17}}}{17} \right) (4) + \left( \frac{2\sqrt{\frac{81}{18}}}{18} \right) (2)
\]

\[
= \left( \frac{8\sqrt{\frac{42}{13}}}{13} + 1 \right) n + \frac{16\sqrt{\frac{20}{9}}}{9} + \frac{4\sqrt{\frac{35}{3}}}{3} + \frac{8\sqrt{\frac{40}{13}}}{13} + \frac{16\sqrt{\frac{3}{7}}}{7} + \frac{8\sqrt{\frac{42}{13}}}{13} + \frac{6\sqrt{\frac{7}{4}}}{4} + \frac{24\sqrt{\frac{2}{17}}}{17} + 9.
\]
(v) The harmonic index:

\[ H^v (H) = \sum_{uv \in E(H)} \frac{2}{\lambda_{uv}(u) + \lambda_{uv}(v)}. \]

\[ H^v (H) = \left( \frac{2}{9} \right) |E_1^v| + \left( \frac{2}{10} \right) |E_2^v| + \left( \frac{2}{12} \right) |E_3^v| + \left( \frac{2}{13} \right) |E_4^v| + \left( \frac{2}{16} \right) |E_5^v| + \left( \frac{2}{17} \right) |E_6^v| + \left( \frac{2}{18} \right) |E_11^v| \]

\[ = \left( \frac{2}{9} \right) (8) + \left( \frac{2}{10} \right) (2) + \left( \frac{2}{12} \right) (8) + \left( \frac{2}{13} \right) (4) + \left( \frac{2}{14} \right) (4n - 4) + \left( \frac{2}{16} \right) (n - 1) + \left( \frac{2}{16} \right) (4) + \left( \frac{2}{18} \right) (2) \]

\[ = \frac{69}{91} H + \frac{42001}{7140}. \]  

(vi) The sum-connectivity index:

\[ \chi^v (H) = \sum_{uv \in E(H)} (\lambda_{uv}(u) + \lambda_{uv}(v))^{-1/2}. \]

\[ \chi^v (H) = \left( 9 \right)^{-1/2} |E_1^v| + \left( 10 \right)^{-1/2} |E_2^v| + \left( 12 \right)^{-1/2} |E_3^v| + \left( 13 \right)^{-1/2} |E_4^v| + \left( 14 \right)^{-1/2} |E_5^v| + \left( 16 \right)^{-1/2} |E_6^v| + \left( 17 \right)^{-1/2} |E_{11}^v| \]

\[ = \left( \frac{1}{\sqrt{9}} \right) (8) + \left( \frac{1}{\sqrt{10}} \right) (2) + \left( \frac{1}{\sqrt{12}} \right) (8) + \left( \frac{1}{\sqrt{13}} \right) (4) + \left( \frac{1}{\sqrt{14}} \right) (4n - 4) + \left( \frac{1}{\sqrt{16}} \right) (n - 1) + \left( \frac{1}{\sqrt{16}} \right) (4) + \left( \frac{1}{\sqrt{18}} \right) (2) \]

\[ = \left( \frac{4}{\sqrt{13}} + \frac{1}{\sqrt{14}} \right) H + \left( \frac{8}{9} + \frac{2}{\sqrt{10}} + \frac{8}{\sqrt{12}} + \frac{4}{\sqrt{14}} - \frac{1}{\sqrt{14}} + \frac{3}{2} + \frac{4}{\sqrt{17}} + \frac{2}{\sqrt{18}} + 1 \right). \]
The ev-degree-based indices. (a) The Zagreb index. (b) The Randic index.

(vii) The Randic index:

\[
R^v (H) = \sum_{uv \in E(H)} \left( \frac{1}{\deg^v(u) \deg^v(v)} \right)^{-(1/2)},
\]

\[
R^v (H) = (20)^{-(1/2)}|E_1^*| + (25)^{-(1/2)}|E_5^*| + (35)^{-(1/2)}|E_3^*| + (40)^{-(1/2)}|E_4^*| + (42)^{-(1/2)}|E_5^*| + (48)^{-(1/2)}|E_6^*| \\
+ (49)^{-(1/2)}|E_7^*| + (63)^{-(1/2)}|E_8^*| + (64)^{-(1/2)}|E_9^*| + (72)^{-(1/2)}|E_{10}^*| + (81)^{-(1/2)}|E_{11}^*|
\]

\[
= \left( \frac{1}{\sqrt{20}} \right) (8) + \left( \frac{1}{\sqrt{25}} \right) (2) + \left( \frac{1}{\sqrt{35}} \right) (8) + \left( \frac{1}{\sqrt{40}} \right) (4) + \left( \frac{1}{\sqrt{42}} \right) (4n - 4) + \left( \frac{1}{\sqrt{48}} \right) (4) \\
+ \left( \frac{1}{\sqrt{49}} \right) (n - 1) + \left( \frac{1}{\sqrt{63}} \right) (4) + \left( \frac{1}{\sqrt{64}} \right) (6) + \left( \frac{1}{\sqrt{72}} \right) (2) + \left( \frac{1}{\sqrt{81}} \right) (2)
\]

\[
= \left( \frac{4}{\sqrt{42}} + \frac{1}{7} \right) n + \left( \frac{4}{\sqrt{5}} + \frac{2}{5} + \frac{8}{\sqrt{35}} + \frac{2}{\sqrt{10}} + \frac{1}{\sqrt{3}} - \frac{4}{\sqrt{42}} - \frac{1}{7} + \frac{4}{3\sqrt{7}} + \frac{2}{3\sqrt{2}} + \frac{2}{4} + \frac{2}{9} \right).
\]

6. Numerical Results and Discussion

The experimental studies have a broad range of applications in the fields of chem-informatics, bio-informatics, and biomedicine, where various graph topological-based assessments are used to tackle many complicated schemes. We have carried out the calculations of the numerical results depending upon the topological indices related to crystallographic molecular structure of multiple segment linear hexagonal chain \( L[m, n] \) and hammer-like benzenoid \( H_n \). We have computed the ev-degree, ve-degree, and end-vertex degree-based topological indices, namely, \( M^{ev}, M^{ve}, M^{bve}, M^{bev}, R^{ev}, R^{ve}, (ve-ABC), (ve-GA), (ve-H), \) and (ve-\( \pi \)). In order to see the physical interpretation of the calculated indices, we have illustrated the results with the help of graphical representations and numerical tables. The results are shown in Figures 3(a)–8 and Tables 7 and 8 for the crystallographic molecular structure of multiple segment linear hexagonal chain \( L[m, n] \) and in the Figure 9 and Tables 9 and 10 for the crystallographic molecular structure of hammer-like benzenoid \( H_n \). It can be seen from Tables 7–10 and the Figures 3–9 that with an increase in \( m \) and \( n \), all the computed topological descriptors gave an increased value.

The Zagreb type indices helped in computing total \( \pi \)-electron energy of molecules [47]; thus, the total \( \pi \)-electron energy is in increasing order for the case of multiple segment linear hexagonal chain \( L[m, n] \) and the hammer-like benzenoid \( H_n \), for higher values of \( m \) and \( n \). The Randic index can be used in the study of the chemical similarity of molecular compounds [48]. Moreover, the Randic index can be used in computing the Kovats constants and boiling point of molecules. The value of randic index increases with increase in the values of \( m \) and \( n \) for
Figure 4: The first Zagreb $\alpha$-index.

Figure 5: (a) The first Zagreb $\beta$-index (I). (b) The second Zagreb index.

Figure 6: (a) The atom-bond connectivity index. (b) The geometric-arithmetic index.
Table 7: Numerical representation of the computed indices for certain values of $m$ and $n$.

| $[m,n]$ | $\mathcal{M}^{\alpha} (H)$ | $\mathcal{R}^{\alpha} (H)$ | $\mathcal{M}^{\beta} (H)_1$ | $\mathcal{R}^{\beta} (H)_1$ | $\mathcal{M}^{\alpha} (H)_2$ | $\mathcal{R}^{\alpha} (H)_2$ |
|--------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| [1, 1] | 98              | 3.0138          | 100             | 48              | 87              |                  |
| [2, 2] | 646             | 11.8299         | 1120            | 316             | 989             |                  |
| [3, 3] | 1738            | 29.4343         | 2820            | 852             | 2787            |                  |
| [4, 4] | 3374            | 55.8272         | 5200            | 1656            | 5481            |                  |
| [5, 5] | 5554            | 91.0085         | 8260            | 2728            | 9071            |                  |
| [6, 6] | 8278            | 134.9782        | 12000           | 4068            | 13557           |                  |
| [7, 7] | 11546           | 187.7363        | 16420           | 5676            | 18939           |                  |
| [8, 8] | 15358           | 249.2828        | 21520           | 7552            | 25217           |                  |
| [9, 9] | 19714           | 319.6177        | 27300           | 9696            | 32391           |                  |
| [10, 10]| 24614           | 398.7411        | 33760           | 12108           | 40461           |                  |

Table 8: Numerical representation of the computed indices for certain values of $m$ and $n$.

| $[m,n]$ | $\text{ABC}^{\alpha} (H)$ | $\text{GA}^{\alpha} (H)$ | $\mathcal{H}^{\alpha} (H)$ | $\chi^{\alpha} (H)$ | $\mathcal{R}^{\alpha} (H)$ |
|--------|-----------------|-----------------|-----------------|-----------------|-----------------|
| [1, 1] | 3.7140          | 0.0455889       | 4.1055          | 2.0997          | 1.4793          |
| [2, 2] | 13.8932         | 0.1053527       | 9.7866          | 7.5981          | 4.5345          |
| [3, 3] | 34.1879         | 0.18506         | 9.7866          | 18.4626         | 18.5669         |
| [4, 4] | 64.5981         | 0.2847113       | 18.4626         | 30.1335         | 19.6550         |
| [5, 5] | 105.1239        | 0.404306        | 30.1335         | 56.9157         | 31.7203         |
| [6, 6] | 155.7651        | 0.543845        | 56.9157         | 84.2957         | 46.7891         |
| [7, 7] | 216.5218        | 0.7033269       | 84.2957         | 117.1461        | 64.8612         |
| [8, 8] | 287.3941        | 0.8827528       | 117.1461        | 155.4669        | 85.9366         |
| [9, 9] | 368.3818        | 1.0821225       | 155.4669        | 213.4110        | 110.0155        |
| [10, 10]| 459.4851        | 1.301436        | 213.4110        | 268.5196        | 137.0977        |
multiple segment linear hexagonal chain $L[m, n]$ and the hammer like benzenoid $H_n$. Moreover, for both structures the GA index also increases with the increase in value of $m$ and $n$. Moreover, GA index for the multiple segment linear hexagonal chains $L[m, n]$ and the hammer-like benzenoid $H_n$ increases with the increment in $m$ and $n$. The atom-bond connectivity (ABC) index provides a very good correlation for computing the strain energy of cycloalkanes as well as for the stability of linear and branched alkanes [49]. The ABC index increases for $L[m, n]$ and $H_n$ with the increase in the values of $m$ and $n$.

Table 9: Numerical representation of the computed indices for certain values of $n$.

| $n$ | $M^{ve}$ ($H$) | $R_{ee}$ ($H$) | $M_1^{ave}$ ($H$) | $M_1^{ave}$ ($H$) | $M_2^{ave}$ ($H$) |
|-----|----------------|----------------|-------------------|-------------------|-------------------|
| [1] | 1136           | 18.6874        | 1468              | 560               | 1928              |
| [2] | 1272           | 20.8845        | 1638              | 626               | 2145              |
| [3] | 1408           | 23.0816        | 1808              | 692               | 2362              |
| [4] | 1544           | 25.2787        | 1978              | 758               | 2579              |
| [5] | 1680           | 27.4758        | 2148              | 824               | 2796              |
| [6] | 1816           | 29.6729        | 2318              | 890               | 3013              |
| [7] | 1952           | 31.8700        | 2488              | 956               | 3230              |
| [8] | 2088           | 34.0671        | 2658              | 1022              | 3447              |
| [9] | 2224           | 36.2642        | 2828              | 1088              | 3664              |
| [10]| 2360           | 38.4613        | 2998              | 1154              | 3881              |

Table 10: Numerical representation of the computed indices for certain values of $n$.

| $n$ | ABC$^{ve}$ ($H$) | GA$^{ve}$ ($H$) | $H^{ve}$ ($H$) | $X^{ve}$ ($H$) | $R_{ee}$ ($H$) |
|-----|-----------------|----------------|---------------|----------------|----------------|
| [1] | 21.9366         | 47.6310        | 6.6407        | 9.9507         | 6.6985         |
| [2] | 24.4785         | 52.6192        | 7.3990        | 11.3274        | 7.4586         |
| [3] | 27.0205         | 57.6073        | 8.1572        | 12.7041        | 8.2186         |
| [4] | 29.5624         | 62.5955        | 8.9155        | 14.0807        | 8.9787         |
| [5] | 32.1043         | 67.5836        | 9.6737        | 15.4574        | 9.7388         |
| [6] | 34.6463         | 72.5718        | 10.4319       | 16.8340        | 10.4988        |
| [7] | 37.1882         | 77.5599        | 11.1902       | 18.2107        | 11.2589        |
| [8] | 39.7302         | 82.5481        | 11.9484       | 19.5874        | 12.0190        |
| [9] | 42.2721         | 87.5362        | 12.7067       | 20.9640        | 12.7791        |
| [10]| 44.8140         | 92.5244        | 13.4649       | 22.3407        | 13.5391        |

Figure 9: (a) $M^{ve}$, $M_1^{ave}$, $M_2^{ave}$, and $M_2^{ave}$. (b) $ABC^{ve}$, $GA^{ve}$, $H^{ve}$, and $X^{ve}$. (c) $R_{ee}$ and $R_{ee}$.
7. Conclusion

The topological index (TI) is a quantitative measure that represents the physical, biological, and chemical behavior of essential organic molecules such as moisture and forming heat; boiling, melting, and flickering point; and temperature, strain, partition coefficient, fluid voltage, density, and molecular weight in chromatography. Graph topologies are important tools for approximating and predicting the properties of biological and chemical compounds in the analysis of the quantitative structure-property relationships (QSPRs) and the quantitative structure-activity relationships (QSARs). In this paper, we have evaluated the ev- and ve-degree-based topological indices with graphical representations for molecular structure of multiple segment linear hexagonal chains $L[m,n]$ and the hammer-like benzenoid $H_n$ to study the pharmaceutical and chemical properties and biological behavior. Further studies are also required for the better understanding of multiple segment linear hexagonal chain $L[m,n]$ and the hammer-like benzenoid $H_n$.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

References

[1] Z.-Q. Cai, A. Rauf, M. Ishtiaq, and M. K. Siddiqui, "On ve-degree and ev-degree based topological properties of silicon carbide Si2C3-II[p, q]," *Polycyclic Aromatic Compounds*, pp. 1–15, 2020.

[2] S. M. Hosamani, B. B. Kulkarni, R. G. Boli, and M. G. Vijay, "QSAR analysis of certain graph theoretical matrices and their corresponding energy," *Applied Mathematics and Nonlinear Sciences*, vol. 2, no. 1, pp. 131–150, 2017.

[3] J.-B. Liu, M. Siddiqui, M. Zahid, M. Naeem, A. Baig, and Q. B. Abdul, "Topological properties of crystallographic structure of molecules," *Symmetry*, vol. 10, no. 7, p. 265, 2018.

[4] Z. Shao, M. Siddiqui, and M. Muhammad, "Computing zagreb indices and zagreb polynomials for symmetrical nanotubes," *Symmetry*, vol. 10, no. 7, p. 244, 2018.

[5] Z. Shao, P. Wu, X. Zhang, D. Dimitrov, and J.-B. Liu, "On the maximum ABC index of graphs with prescribed size and without pendant vertices," *IEEE Access*, vol. 6, pp. 27604–27616, 2018.

[6] R. Gozalbes, J. P. Doucet, and F. Derouin, "Application of topological descriptors in QSAR and drug design: history and new trends," *Current Drug Targets- Infectious Disorders*, vol. 2, no. 1, pp. 93–102, 2002.

[7] C. Nantasenamat, C. Isaranurak-Na-Ayudhya, T. Naenna, and V. Prachayasittikul, A Practical Overview of Quantitative Structure-Activity Relationship. 2009.

[8] C. Nantasenamat, C. Isaranurak-Na-Ayudhya, and V. Prachayasittikul, "Advances in computational methods to predict the biological activity of compounds," *Expert Opinion on Drug Discovery*, vol. 5, no. 7, pp. 633–654, 2010.

[9] M. Faraday, "XX On new compounds of carbon and hydrogen, and on certain other products obtained during the decomposition of oil by heat," *Philosophical Transactions of the Royal Society of London*, vol. 115, pp. 440–466, 1825.

[10] R. Kaiser, "Bicarburet of hydrogen Reappraisal of the discovery of benzene in 1825 with the analytical methods of 1968," *Angewandte Chemie International Edition in English*, vol. 7, no. 5, pp. 345–350, 1968.

[11] E. Mitscherlich, "Ueber das Benzol und die Säuren der Oel- und Talgarten," *Annalen der Pharmacie*, vol. 9, no. 1, pp. 39–48, 1834.

[12] A. W. Hofmann, "Ueber eine sichere Reaction auf Benzol," *Annalen der Chemie und Pharmacie*, vol. 55, no. 2, pp. 200–205, 1845.

[13] A. Kekulé, "Sur la constitution des substances aromatiques," *Bulletin mensuel de la Société Chimique de Paris*, vol. 3, p. 98, 1865.

[14] US Department of Health and Human Services, Agency for Toxic Substances and Disease registry Toxicological Profile for Lead, 2007.

[15] H. Wiener, "Structural determination of paraffin boiling points," *Journal of the American Chemical Society*, vol. 69, no. 1, pp. 17–20, 1947.

[16] L. I. Stiel and G. Thodos, "The normal boiling points and critical constants of saturated aliphatic hydrocarbons," *AIChE Journal*, vol. 8, no. 4, pp. 527–529, 1962.

[17] D. H. Rouvray and B. C. Crafford, "Dependence of physicochemical properties on topological factors," *South African Journal of Science*, vol. 72, no. 2, pp. 47–51, 1976.

[18] Y. Ma, S. Cao, Y. Shi, I. Gutman, M. Dehmer, and B. Furtula, "From the connectivity index to various Randić-type descriptors," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 80, no. 1, pp. 85–106, 2018.

[19] A. Ali, I. Gutman, E. Milovanovic, and I. Milovanovic, "Sum of powers of the degrees of graphs: extremal results and bounds," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 80, no. 1, pp. 5–84, 2018.

[20] B. Borovicanin, K. C. Das, B. Furtula, and I. Gutman, "Bounds for zagreb indices," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 78, no. 1, pp. 17–100, 2017.

[21] I. Gutman, E. Milovanović, and I. Milovanović, "Beyond the Zagreb indices," *AKCE International Journal of Graphs and Combinatorics*, vol. 17, no. 1, pp. 74–85, 2020.

[22] L. Zhong, "The harmonic index for graphs," *Applied Mathematics Letters*, vol. 25, no. 3, pp. 561–566, 2012.

[23] M. Chellali, T. W. Haynes, S. T. Hedetniemi, and T. M. Lewis, "On ve-degrees and ev-degrees in graphs," *Discrete Mathematics*, vol. 340, no. 2, pp. 31–38, 2017.

[24] B. Horoldagva, K. C. Das, T. A. D. Selenge, and A. S. Tsend, "On ve-Degree and ev-Degree of Graphs," *Discrete Optimization*, vol. 31, pp. 1–7, 2019.

[25] A. Rauf, M. Ishtiaq, M. K. Siddiqui, and R. Andleeb, "Topological properties of doxorubicin conjugated PEG-PAsp copolymer molecular structure used in cancer treatment," *Polycyclic Aromatic Compounds*, pp. 1–14, 2020.

[26] Y.-M. Chu, M. K. Siddiqui, F. H. Muhammad et al., "On ve-degree and ev-degree based topological properties of H-naphthalene nanotube," *Polycyclic Aromatic Compounds*, pp. 1–13, 2020.

[27] X. Zhang, A. Rauf, M. Ishtiaq, M. K. Siddiqui, and M. H. Muhammad, "On degree based topological properties..."
of two carbon nanotubes,” *Polycyclic Aromatic Compounds*, pp. 1–19, 2020.

[29] Z.-Q. Cai, A. Rauf, M. Ishtiaq, and M. K. Siddiqui, “On ve-degree and ev-degree based topological properties of silicon carbide Si2C3-II[p, q],” *Polycyclic Aromatic Compounds*, pp. 1–15, 2020.

[30] A. Rauf, M. Ishtiaq, and M. K. Siddiqui, “Topological study of hydroxychloroquine conjugated molecular structure used for novel coronavirus (COVID-19) treatment,” *Polycyclic Aromatic Compounds*, vol. 18, pp. 1–17, 2020.

[31] A. Ye, M. I. Qureshi, A. Fahad et al., “Zagreb connection number index of nanotubes and regular hexagonal lattice,” *Open Chemistry*, vol. 17, no. 1, pp. 75–80, 2019.

[32] Z. Iqbal, A. Aslam, M. Ishtiaq, and W. Gao, “The edge versions of degree-based topological descriptors of dendrimers,” *Journal of Cluster Science*, vol. 31, no. 2, pp. 445–452, 2019.

[33] A. Aslam, Y. Bashir, M. Rafiq et al., “Three new/old vertex-degree-based topological indices of some dendrimers structure,” *Electronic Journal of Biology*, vol. 13, no. 1, pp. 94–99, 2017.

[34] M. Berhe Belay and C. Wang, “The first general Zagreb coindex of graph operations,” *Applied Mathematics and Nonlinear Sciences*, vol. 5, no. 2, pp. 109–120, 2020.

[35] S. Shirakol, M. Kalyanshetti, and S. M. Hosamani, “QSPR analysis of certain distance based topological indices,” *Applied Mathematics and Nonlinear Sciences*, vol. 4, no. 2, pp. 371–386, 2019.

[36] M. Berhe and C. Wang, “Computation of certain topological coindices of graphene sheet and C 4 C 8(S) nanotubes and nanotorus,” *Applied Mathematics and Nonlinear Sciences*, vol. 4, no. 2, pp. 455–468, 2019.

[37] S. Goyal, P. Garg, and V. N. Mishra, “New composition of graphs and their Wiener Indices,” *Applied Mathematics and Nonlinear Sciences*, vol. 4, no. 1, pp. 163–168, 2019.

[38] A. u. R. Virk, T. Abbas, and W. Khalid, “Multiplicative topological descriptors of Silicon carbide,” *Applied Mathematics and Nonlinear Sciences*, vol. 4, no. 1, pp. 181–190, 2019.

[39] A. Portilla, J. M. Rodriguez, and J. M. Sigaretta, “Recent lower bounds for geometric-arithmetic index,” *Discrete Mathematics Letters*, vol. 1, pp. 59–82, 2019.

[40] A. Ali, L. Zhong, and I. Gutman, “Harmonic index and its generalizations: extremal results and bounds,” *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 81, no. 2, pp. 249–311, 2019.

[41] M. T. Smith, “Advances in understanding benzene health effects and susceptibility,” *Annual Review of Public Health*, vol. 31, pp. 133–148, 2010.

[42] C. G. Santesson, “Uber chronische vergiftung mit steinkohle-lenteerbrenzin: vier todesfälle,” *Air Hygiene in Dressing-Rooms For Burns*, vol. 31, p. 336, 1897.

[43] H. G. Weiskotten, C. B. Gibbs, E. O. Boggs, and E. R. Templeton, “The action of benzol: VI. Benzol vapor leucopenia (rabbit),” *The Journal of Medical Research*, vol. 41, no. 4, pp. 425–38, 1920.

[44] H. G. Weiskotten, S. C. Shwartz, and H. S. Steinsland, “The action of benzol on blood and blood forming tissues,” *The Journal of Medical Research*, vol. 35, pp. 63–69, 1916.

[45] L. Selling, *Benzol as a Leucotoxin: Studies on the Degeneration and Regeneration of the Blood and Haematopoietic Organs*, Johns Hopkins Press, Baltimore, Maryland, USA, 1913.

[46] I. Gutman and J. Sven, *Cyvin. Introduction to the Theory of Benzenoid Hydrocarbons*, Springer Science & Business Media, Berlin, Germany, 2012.