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Research Article

Some Bounds on Bond Incident Degree Indices with Some Parameters

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It is considered that there is a fascinating issue in theoretical chemistry to predict the physicochemical and structural properties of the chemical compounds in the molecular graphs. These properties of chemical compounds (boiling points, melting points, molar refraction, acentric factor, octanol-water partition coefficient, and motor octane number) are modeled by topological indices which are more applicable and well-used graph-theoretic tools for the studies of quantitative structure-property relationships (QSPRs) and quantitative structure-activity relationships (QSARs) in the subject of cheminformatics. The π-electron energy of a molecular graph was calculated by adding squares of degrees (valencies) of its vertices (nodes). This computational result, afterwards, was named the first Zagreb index, and in the field of molecular graph theory, it turned out to be a well-swotted topological index. In 2011, Vukicevic introduced the variable sum exdeg index which is famous for predicting the octanol-water partition coefficient of certain chemical compounds such as octane isomers, polyaromatic hydrocarbons (PAH), polychlorobiphenyls (PCB), and phenethylamines (Phenet). In this paper, we characterized the conjugated trees and conjugated unicyclic graphs for variable sum exdeg index in different intervals of real numbers. We also investigated the maximum value of SEIa for bicyclic graphs depending on $a > 1$.

1. Introduction

In chemical graph theory, molecules and macromolecules (such as organic compounds, nucleic acids, and proteins) are represented by graphs wherein vertices correspond to the atoms, whereas edges represent the bonds between atoms [1, 2]. A topological index is a numerical value associated with chemical constitution for correlation of chemical structure with various physicochemical properties [3]. Topological indices play a significant role in organic chemistry and particularly in pharmacology [4, 5]. Physicochemical properties of chemical compounds such as relative enthalpy of formation, biological activity, boiling points, melting points, molar refraction, acentric factor, octanol-water partition coefficient, and motor octane number are modeled by topological indices in quantitative structure-property relation (QSPR) and quantitative structure-activity relation (QSAR) studies [4, 6–8].

In chemistry, the usage of topological index started in 1947 when the chemist Wiener developed the Wiener index (a distance-based topological index) to predict boiling points of paraffins [9]. Platt index (the oldest degree-based topological index) was proposed in 1952 for predicting paraffin properties [10]. The π-electron energy of a molecular graph was calculated by adding square of degrees (valencies) of its vertices (nodes) in the year 1972. The same computational result, afterwards, was named the first Zagreb index, and in the field of molecular graph theory, it turned out to be a well-swotted topological index [11]. For more details about the topological indices in the field of chemistry, we refer to [6, 8, 12–15].

Many well-known topological indices such as hyper Zagreb index [16], variable sum exdeg index [17], and Zagreb indices [18, 19] have been used to find out sharp bounds for unicyclic, bicyclic, and tricyclic graphs. Vukicevic [15] propounded variable sum exdeg index for a graph G and defined it as

$$\mathrm{SEI}_a(G) = \sum_{uv\in E(G)} \left(a^{d_u} + a^{d_v}\right) = \sum_{u\in V(G)} \left(d_u a^{d_u}\right), \tag{1}$$

where a is a positive integer other than 1. This topological index is correlated well with octane-water partition coefficient [15] and is employed to the study of octane isomers (see [20–22]). This topological index in the form of polynomial was proposed by Yarahmadi and Ashrafi, and they find its application in nanoscience [23]. Chemical application of this index can be seen in the papers [12, 13, 15].

In this paper, we mainly targeted three main problems. First of all, we find the extremal values of variable sum exdeg index (SEI_a) for conjugated trees. After that, we investigated lower and upper bounds of unicyclic conjugated graphs with respect to the length of this cycle in different intervals. At the end of this paper, we find upper bounds of SEI_a for bicyclic graphs. This paper contains seven sections. In the first section, we have given introduction while in Section 2, we have given the proofs of some lemmas and preliminary results. In Section 3, we discovered the bounds of a conjugated trees and this section helps us to find out lower and upper bounds of unicyclic conjugated graphs with respect to the length of this cycle in Section 4. In Section 5, we discussed an important theorem related with conjugated unicyclic graphs. In Section 6, we discovered the upper bounds of bicyclic graphs. In the last section, we have drawn the conclusion.

2. Preliminary Results

All graphs under consideration in this paper will be connected, simple, and finite. Suppose $G = (V(G), E(G))$ is a simple and finite graph, whereas set of vertices is denoted by $V(G)$ and the set of edges is denoted by $E(G)$. Let $v \in V(G)$ for which d_v is defined as the cardinality of edges incident with the vertex v. Suppose $N_G(v)$ denotes the set of all vertices which are adjacent with the vertex v and $N_G[v] = N_G(v) \bigcup \{v\}$. Note that $\Delta(G)$ and $\delta(G)$ represent the maximum and minimum degree of a graph G, respectively. A pendent vertex is a vertex of degree one. An edge whose one end is a pendent vertex is called pendent edge. Let $B \subseteq V(G)$ and $B' \subseteq E(G)$; then, $G - B$ and $G - B'$ are subgraphs of G which are obtained by deleting the vertices and edges from G, respectively. An edge between the vertices x and y is denoted by $e = xy$. If $B = \{v\}$ and $B' = \{xy\}$, then $G - B$ and $G - B'$ can be expressed as $G - v$ and $G - xy$, respectively.

In a graph G, if the vertices x and y are nonadjacent, then $G + xy$ means there is an addition of an edge between the vertices x and y in a graph G. We use S_n, C_n, and P_n to denote the star graph, cycle graph, and path graph on n vertices, respectively. We assume that graphs (G^*, w_1) and (G^{**}, w_2) be rooted at w_1 and w_2, respectively. Then, $(G^*, w_1) \Cup (G^{**}, w_2)$ is obtained by identifying w_1 and w_2 as the same vertex. A graph which has no cycle is called a tree. A graph G is said to be unicyclic graph if it has a unique cycle. A graph G is said to be bicyclic graph if G has exactly $n+1$ edges. Let $\mathbb{U}_l(n)$ represent the collection of all those graphs which have order n and a unique cycle of length l. We denote $\mathbb{U}_l(2m, m)$ the collection of all conjugated unicyclic graphs of order n in which length of its cycle is l, whereas m is the matching number of G. Let $G \in \mathbb{U}_l(2m, m)$ be a unicyclic graph of length l and it is denoted by C_l. Let $G \in \mathbb{U}_l(2m, m)$; if $n = 2m = l$ or $n = 2m = l + 1$, then its $\mathrm{SEI}_a(G)$ is unique. That is why in this paper we will assume $n = 2m \geq l + 2$. One can find terminologies and expressions "indefinito" in [24–26].

Suppose that G' is a graph acquired from another graph G by using some graph alteration such that $V(G) = V(G')$. In all sections of this paper, whenever such two graphs are under debate, we always mean the vertex degree d_x the degree of the vertex x in G.

Lemma 1. *Let G be a graph of order n if G contains the vertices $u, v \in V(G)$ such that $d_u = s > 1$, $d_v = t > 1$ and $s \geq t$; then, there exists a graph G' such that $\mathrm{SEI}_a(G') > \mathrm{SEI}_a(G)$ for $a > 1$.*

Proof. Let $u, v \in V(G)$ and $v_1, v_2, v_3, \ldots v_k$ be the pendent vertices adjacent to the vertex v. We define a new graph G', i.e., $G' = G - \{v_1v, v_2v, \ldots, v_kv\} + \{v_1u, v_2u, \ldots, v_ku\}$ as in Figure 1. By the definition of $\mathrm{SEI}_a(G)$, we have

$$\begin{aligned}\mathrm{SEI}_a(G) - \mathrm{SEI}_a(G') &= \left[d_u.a^{d_u} + d_v.a^{d_v}\right] - \left[(d_u + k).a^{d_u+k} + (d_v - k).a^{d_v-k}\right]\\ &= \left[d_v.a^{d_v} - (d_v - k).a^{d_v-k}\right] - \left[(d_u + k).a^{d_u+k} - d_u.a^{d_u}\right]\\ &= k\left[a^{\mu_1}(1 + \mu_1 \ln a) - a^{\mu_2}(1 + \mu_2 \ln a)\right] < 0,\end{aligned} \tag{2}$$

where $\mu_1 \in (t - k, t)$, $\mu_2 \in (s, s + k)$, $\mu_2 > \mu_1$ for $a > 1$. Thus, the proof of the above lemma is accomplished. □

Lemma 2. *Let G be a graph having two components G_1 and T_1, where G_1 is a cycle graph and T_1 is a star graph with*

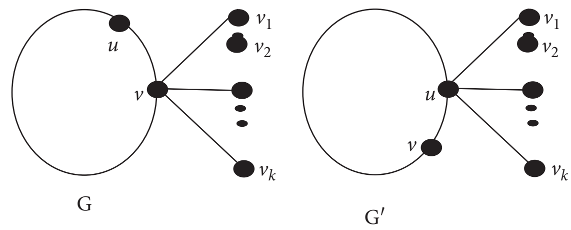

Figure 1: (a) G and (b) G′ is constructed from G.

central vertex v. Let $u \in V(G_1)$ *and* $d_u = p$*, such that uv is an edge in G. Let* $v_1, v_2, v_3, \ldots v_k$ *be the pendent vertices adjacent with the vertex v, i.e.,* $N_G(v) - \{u\} = \{v_1, v_2, v_3, \ldots, v_k\}$*. We define* $G' = G - \{v_1v, v_2v, \ldots, v_kv\} + \{v_1u, v_2u, \ldots, v_ku\}$ *such that* $SEI_a(G') > SEI_a(G)$*.*

Proof. Let G be a graph having two components $G_1$and T_1 where G_1 is a cycle graph and T_1 is a star graph with central vertex v. Let $u \in V(G_1)$, $d_u = p$, such that uv is an edge in G. Let $v_1, v_2, v_3, \ldots v_k$ be the pendent vertices adjacent with the vertex v, i.e., $N_G(v) - \{u\} = \{v_1, v_2, v_3, \ldots v_k\}$. We define $G' = G - \{v_1v, v_2v, \ldots, v_kv\} + \{v_1u, v_2u, \ldots, v_ku\}$ as in Figure 2. By the definition of SEI_a, we have

$$\begin{aligned}\mathrm{SEI}_a(G) - \mathrm{SEI}_a(G') &= \left[d_u.a^{d_u} + d_v.a^{d_v}\right] - \left[(d_u + k).a^{d_u+k} + (d_v - k).a^{d_v-k}\right]\\ &= \left[d_v.a^{d_v} - (d_v - k).a^{d_v-k} - \left[(d_u + k).a^{d_u+k} - d_u.a^{du}\right].\end{aligned} \tag{3}$$

If $p \geq k + 1$, then

$$\begin{aligned}\mathrm{SEI}_a(G) - \mathrm{SEI}_a(G') &= \left[d_v.a^{d_v} - (d_v - k).a^{d_v-k}\right]\\ &\quad - \left[(d_u + k).a^{d_u+k} - d_u.a^{du}\right]\\ &= k\left[a^{\mu_1}(1 + \mu_1 \ln a) - a^{\mu_2}(1 + \mu_2 \ln a)\right] < 0,\end{aligned} \tag{4}$$

where $\mu_1 \in (1, k + 1)$, $\mu_2 \in (p, p + k)$, $\mu_2 > \mu_1$, and $a > 1 \mathrm{SEI}_a(G') > \mathrm{SEI}_a(G)$.

If $p \leq k + 1$, then

$$\begin{aligned}\mathrm{SEI}_a(G) - \mathrm{SEI}_a(G') &= \left[d_u.a^{du} - (d_v - k).a^{d_v-k}\right]\\ &\quad - \left[(d_u + k).a^{d_u+k} - d_v.a^{d_v}\right]\\ &= z.\left[a^{\mu_1}(1 + \mu_1 \ln a) - a^{\mu_2}(1 + \mu_2 \ln a)\right] < 0,\end{aligned} \tag{5}$$

where $\mu_1 \in (1, p)$, $\mu_2 \in (k + 1, k + p)$, $\mu_2 > \mu_1$, $z = p - 1$ and $a > 1$. Thus, we have $\mathrm{SEI}_a(G') > \mathrm{SEI}_a(G)$. □

3. Extremal Values of Variable Sum Exdeg Index for Conjugated Trees

First we introduce some notations which will be used in the following lemmas and theorems. Suppose that $\mathbb{T}(n, m)$ be the collection of all trees with n vertices and m-matching number with $n \geq 2m$. When $m - 1$ pendent vertices are attached with each certain non-central vertices of S_{n-m+1}, then the resulting graph is denoted by $\mathbb{T}^0(n, m)$. If we choose $n = 2m$, then it means every tree from $\mathbb{T}(n, m)$ and $\mathbb{T}^0(n, m)$ contains perfect matching.

Lemma 3 (see [26]). *If an n-vertex tree T has perfect matching, then there must exist at least two vertices of degree one with neighbouring vertices of degree two, where* $n \geq 3$*.*

Lemma 4 (see [26]). *If an n-vertex tree T has an m-matching with* $n > 2m$*, then there must exist a pendent vertex u which is not saturated by m-matching.*

In the following, we will find two theorems which will give extreme values of SEI_a for all trees T in $\mathbb{T}(2m, m)$.

Theorem 1. *Let* $m \geq 1$*,* $n \geq 4$*, and* $a > 1$ *be integers and* $T \in \mathbb{T}(2m, m)$*; then,* $SEI_a(T) \leq m.a^m + 2(m - 1)a^2 + am$*, where equality meets when* $T \cong \mathbb{T}^0(2m, m)$*.*

Proof. Suppose $T \in \mathbb{T}(2m, m)$. If the tree T is isomorphic to $\mathbb{T}^0(2m, m)$, then $\mathrm{SEI}_a(T) = \mathrm{SEI}_a(\mathbb{T}^0(2m, m))$. On the other hand, if T is not isomorphic to $\mathbb{T}^0(2m, m)$, then we assume that the vertex $u \in V(T)$, i.e., $d_u = \Delta(T)$ where $d_u \geq 2$. Lemma 3 assures that there exist vertices u_1 and v_1 adjacent by an edge with $d_{u_1} = 2$ and $d_{v_1} = 1$. Let $N(u_1) - \{v_1\} = w_1$. We define $T^{(1)} = T - u_1w_1 + u_1u$. It is clear that $T^{(1)} \in \mathbb{T}(2m, m)$. By the definition of SEI_a, we have

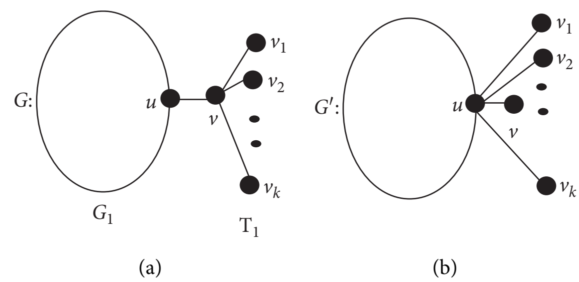

Figure 2: (a) Graph G; (b) the graph G′ is obtained from G.

$$\begin{aligned}\mathrm{SEI}_a(T)-\mathrm{SEI}_a\left(T^{(1)}\right)&=\left[d_u.a^{d_u}+d_{w_1}.a^{d_{w_1}}\right]\\&\quad-\left[\left(d_u+1\right).a^{d_u+1}+\left(d_{w_1-1}\right).a^{\left(d_{w_1-1}\right)}\right]\\&=\left[d_{w_1}.a^{d_{w_1}}-\left(d_{w_1-1}\right).a^{\left(d_{w_1-1}\right)}\right]\\&\quad-\left[\left(d_u+1\right).a^{d_u+1}-d_u.a^{d_u}\right]\\&=a^{\mu_1}\left(1+\mu_1\ln a\right)-a^{\mu_2}\left(1+\mu_2\ln a\right)<0,\end{aligned}\tag{6}$$

where $\mu_1\in(d_{w_1}-1,d_{w_1})$, $\mu_2\in(d_u,\ d_u+1)$, and $\mu_2>\mu_1$ for $a>1$.

Note that $T^*=T^1-\{u_1,v_1\}$; then, obviously $T^*\in\mathbb{T}(2(m-1),m-1)$. Then, by the construction of T^* and keeping Lemma 3 in our mind, we can choose u_2 and v_2 in T^* where $d_{u_2}=2$ and $d_{v_2}=1$. It is clear that $d_u(T^*)=\Delta(T)=\Delta(T^*)$. Let $N(u_2)-\{v_2\}=w_2$. We set $T^{**}=T^*-u_2w_2+u_2u$. Similarly, $\mathrm{SEI}_a(T^{**})>\mathrm{SEI}_a(T^*)$. We define $T^2=T^1-u_2w_2+u_2u$; then,

$$\begin{aligned}\mathrm{SEI}_a\left(T^{(2)}\right)-\mathrm{SEI}_a\left(T^{(1)}\right)&=\left[\left(d_u+2\right).a^{d_u+2}+\left(d_{w_2}-1\right).a^{d_{w_2}-1}\right]\\&\quad-\left[\left(d_u+1\right).a^{d_u+1}+d_{w_2}.a^{d_{w_2}}\right]\\&=\left[\left(d_u+2\right).a^{d_u+2}-\left(d_u+1\right).a^{d_u+1}\right]\\&\quad-\left[d_{w_2}.a^{d_{w_2}}-\left(d_{w_2}-1\right).a^{d_{w_2}-1}\right]\\&=a^{\mu_4}\left(1+\mu_4\ln a\right)-a^{\mu_3}\left(1+\mu_3\ln a\right)>0,\end{aligned}\tag{7}$$

where $\mu_3\in(d_{w_2}-1,d_{w_2}),\mu_4\in(d_u+1,d_u+2)$, and $\mu_4>\mu_3$ for $a>1$.

This implies that $\mathrm{SEI}_a(T^{(2)})-\mathrm{SEI}_a(T^{(1)})>0$. We repeat the above process on the graph T again and again and we obtain a sequence of graphs $T^1,T^2,\ldots,T^{(s)},\ldots$ with the relation $\mathrm{SEI}_a(T^{(1)})<\mathrm{SEI}_a(T^{(2)})<\ldots\mathrm{SEI}_a(T^{(s)})<\ldots$

For some positive integer$p$, we have $T^{(p)}\cong T^{(p+1)}$ and $T^{(p)}\cong(\mathbb{T}^0(2m,m))$.

Hence, $\mathrm{SEI}_a(T)<\mathrm{SEI}_a(\mathbb{T}^0(2m,m))$. □

Theorem 2. *Suppose that $m\geq 1$, $n\geq 4$, and $a>1$ be integers. If $T\in\mathbb{T}(2m,m)$, then $SEI_a(T)\geq 2a+2(2m-2)a^2$, where equality meets when $T\cong P_{2m}$.*

Proof. We claim that $T\cong P_{2m}$; then, $\mathrm{SEI}_a(T)=\mathrm{SEI}_a(P_{2m})$. If we apply the above-defined process (in previous Theorem 1) on T, then we will obtain the expression $\mathrm{SEI}_a(T^{(1)})<\mathrm{SEI}_a(T^{(2)})<\ldots\mathrm{SEI}_a(T^{(s)})<\ldots$ for some positive integer $p\geq 1\mathrm{SEI}_a(T)^p>\mathrm{SEI}_a(P_{2m})$. Hence, $\mathrm{SEI}_a(T)\geq\mathrm{SEI}_a(P_{2m})=2a+2(2m-2)a^2$ equality meets when $T\cong P_{2m}$. □

4. Extremal Values of Variable Sum Exdeg Index for Conjugated Unicyclic Graphs

In this portion of the paper, we will find extreme values for $\mathrm{SEI}_a(G)$ among all the conjugated unicyclic graphs in $\mathbb{U}_l(2m,m)$ for $a>1$. In this concern, we will prove some lemmas which will support our main theorems.

Lemma 5 (see [26]). *For any tree T from $T(2m+1,m)$, we find at least one vertex of degree 1 which will be adjacent with a vertex v of degree 2, i.e., $d_v=2$.*

Lemma 6. *Suppose that $m\geq 1,a>1$ and $T\in T(2m+1,m)$; then, $SEI_a(T)\geq SEI_a(P_{2m+1})$, where sign of equality meets when $T\cong P_{2m+1}$.*

Proof. Let $T\in T(2m+1,m)$; then, by Lemma 4, we find a pendent vertex u in T which is not saturated by an m-matching of T. Obviously, the vertices in $T-\{u\}$ are saturated by the maximal m−matching. This implies that $T-\{u\}\in T(2m,m)$. Assume that $N(u)=\{w\}$; then, $\mathrm{SEI}_a(T)=\mathrm{SEI}_a(T-\{u\})+d_wa^{d_w}+d_ua^{d_u}-(d_w-1)a^{d_w-1}$. According to Theorem 2, we have

$$\begin{aligned}\mathrm{SEI}_a(T)&\geq\mathrm{SEI}_a(P_{2m})+d_wa^{d_w}+a-(d_w-1)a^{d_w-1}\\&=2a+2(2m-2)a^2+d_wa^{d_w}+a-(d_w-1)a^{d_w-1}\\&=2a+2(2m-1)a^2-2a^2+d_wa^{d_w}+a-(d_w-1)a^{d_w-1}\\&\geq 2a+2(2m-1)a^2\\&=\mathrm{SEI}_a(P_{2m+1}).\end{aligned}\tag{8}$$

The above inequality holds if $d_wa^{d_w}-(d_w-1)a^{d_w-1}-(2a^2-a)\geq 0$.

If $d_w=2$, then

$$d_wa^{d_w}-(d_w-1)a^{d_w-1}-\left(2a^2-a\right)=0.\tag{9}$$

If $d_w\geq 3$, then we have

$$a^{\mu_2}(1+\mu_2 \ln a) - a^{\mu_1}(1+\mu_1 \ln a) > 0, \tag{10}$$

where $\mu_1 \in (1,2), \mu_2 \in (d_w - 1, d_w)$, and $\mu_2 > \mu_1$ for $a > 1$. Finally, we have $\mathrm{SEI}_a(T) \geq \mathrm{SEI}_a(P_{2m+1})$. □

Lemma 7. *Let $T \in \mathbb{T}(2m+1,m)$; then, $SEI_a(T) \leq SEI_a(\mathbb{T}^0(2m+1,m))$ equality meets when $T \cong \mathbb{T}^0(2m+1,m)$ where $m \geq 1$, $a > 1$.*

Proof. Let $T \in \mathbb{T}(2m+1,m)$; then, by Lemma 4, we find a pendent vertex u in T which is not saturated by a maximal m'-matching of T. Suppose that $N(u) = \{z_1\}$. Suppose v is a vertex in T, i.e., $d_v = \Delta(T)$. Define $T' = T - uz_1 + uv$; then, clearly $T' - \{u\} \in \mathbb{T}(2m,m)$. With the help of Theorem 1, we have $\mathrm{SEI}_a(T') - \{u\} \leq \mathrm{SEI}_a(\mathbb{T}^0(2m,m))$, so we have

$$\begin{aligned}
\mathrm{SEI}_a(T') &= \mathrm{SEI}_a(T'-u) + d_u a^{d_u} + (d_v+1)a^{d_v+1} - d_v a^{d_v}\\
&\leq a + \mathrm{SEI}_a\left(\mathbb{T}^0(2m,m)\right) + (d_v+1)a^{d_v+1} - d_v a^{d_v}\\
***&< a + \mathrm{SEI}_a\left(\mathbb{T}^0(2m,m)\right) + (m+1)a^{m+1} - ma^m\\
&= a + ma^m + 2a^2(m-1) + a.m + (m+1)a^{m+1} - ma^m\\
&= a + ma^m + 2a^2(m-1) + a.m + (m+1)a^{m+1} - ma^m\\
&= 2a^2(m-1) + (1+m)a + (m+1)a^{m+1}\\
&= \mathrm{SEI}_a\left(\mathbb{T}^0(2m+1,m)\right).
\end{aligned} \tag{11}$$

If we show that $(d_v+1)a^{d_v+1} - d_v a^{d_v} < (m+1)a^{m+1} - ma^m$, then it will be enough for the existence of the expression $***$. Since we know that $\Delta(\mathbb{T}^0(2m,m)) = m$, T is not isomorphic to $\mathbb{T}^0(2m+1,m)$ and $d_v \leq m$. If we assume $d_v = m$, then $(d_v+1)a^{d_v+1} - d_v a^{d_v} - (m+1)a^{m+1} + ma^m = 0$. If we assume $d_v < m$, then

$$\begin{aligned}
&= \left[(d_v+1)a^{d_v+1} - d_v a^{d_v}\right] - \left[(m+1)a^{m+1} - ma^m\right]\\
&= a^{\mu_1}(1+\mu_1 \ln a) - a^{\mu_2}(1+\mu_2 \ln a) < 0,
\end{aligned} \tag{12}$$

where $\mu_1 \in (d_v, d_v+1), \mu_2 \in (m, m+1), \mu_2 > \mu_1$ and $a > 1$.

Hence, $\mathrm{SEI}_a(T) < \mathrm{SEI}_a(T') < \mathrm{SEI}_a(\mathbb{T}^0(2m+1,m))$. So, we conclude that $\mathrm{SEI}_a(T) \leq \mathrm{SEI}_a(\mathbb{T}^0(2m+1,m))$, and sign of equality meets when $T \cong \mathbb{T}^0(2m+1,m)$.

We define a set $B = \{x_i \in V(C_l)\colon d_{x_i} \geq 3\}$. Remember that $T(x_i)$ represents the connected component having the vertex x_i of the graph $G - \{x_{i-1}x_i, x_i x_{i+1}\}$. □

Lemma 8 (see [26]). *Let $G \in \mathbb{U}_l(2m,m)$; then, for every $x_i \in B$, $T(x_i) \in T(n_i, n_i/2)$ or $T(x_i) \in T(n_i, n_i - 1/2)$.*

Lemma 9. *Let $G \in \mathbb{U}_l(2m,m)$ such that $SEI_a(G)$ is minimum if $T(x_i) \cong P_{n_i}$ where $x_i \in B, n_i = n(T(x_i)), a > 1$ and x_i is one of the pendent vertices of P_{n_i}.*

Proof. Suppose $G \in \mathbb{U}_l(2m,m)$ with minimum variable sum exdeg index. We also assume that $x_i \in B$ and the vertices x_{i-1} and x_{i+1} are the neighbouring vertices of the vertex x_i along C_l. Here we consider the expression

$$\begin{aligned}
Q &= \left[d_{x_i}a^{d_{x_i}} - \left(d_{x_i}-2\right)a^{d_{x_i}-2}\right] + \left[d_{x_{i-1}}a^{d_{x_{i-1}}} - \left(d_{x_{i-1}}-1\right)a^{d_{x_{i-1}}-1}\right]\\
&\quad + \left[d_{x_{i+1}}a^{d_{x_{i+1}}} - \left(d_{x_{i+1}}-1\right)a^{d_{x_{i+1}}-1}\right].
\end{aligned} \tag{13}$$

We assume that G^* is the connected component of $G - \{x_i x_{i-1}, x_i x_{i+1}\}$ which does not contain the vertex x_i. We can write the expression, $\mathrm{SEI}_a(G) = \mathrm{SEI}_a(G^*) + Q + \mathrm{SEI}_a(T_{x_i})$. According to Lemma 8, $T(x_i) \in T(n_i, n_i/2)$ or $T(x_i) \in T(n_i, n_i - 1/2)$. In either situation, there exists the following relation: $\mathrm{SEI}_a(G) \geq \mathrm{SEI}_a(G^*) + Q + \mathrm{SEI}_a(P_{n_i})$ according to Theorem 2 and Lemma 6. Furthermore, the sign of equality meets iff $T(x_i) \cong P_{n_i}$. Next we will prove that the vertex x_i is one of the pendent vertices of P_{n_i} such that $d_{x_i} = 3$. We suppose that $d_{x_i} \geq 4$, so there must exist two vertices u and v, i.e., $N(x_i) - \{x_{i-1}, x_{i+1}\} = \{u, v\}$. Then, there must be one edge of $x_i u$, or $x_i v$ which is not included in m-matching. Without loss of generality, suppose that $x_i u$ does not belong to the m-matching. Let $P(v) = v_1, v_2, \ldots v_q$ where $q \geq 2$ represents the path with $v = v_1$ as a pendent vertex of $P(v)$. Define $G' = G - x_i u + uv_q$; it is clear that $G' \in U_l(2m,m)$. By the definition of SEI_a, we have

$$\begin{aligned}
\mathrm{SEI}_a(G') - \mathrm{SEI}_a(G) &= \left[\left(d_{x_i}-1\right)a^{d_{x_i}-1} + \left(d_{v_q}+1\right)a^{d_{v_q}+1}\right]\\
&\quad - \left[\left(d_{x_i}\right)a^{d_{x_i}} + d_{v_q}a^{d_{v_q}}\right]\\
&= \left[\left(d_{v_q}+1\right)a^{d_{v_q}+1} - \left(d_{v_q}\right)a^{d_{v_q}}\right]\\
&\quad - \left[d_{x_i}a^{d_{x_i}} - \left(d_{x_i}-1\right)a^{d_{x_i}-1}\right]\\
&= a^{\mu_1}(1+\mu_1 \ln a) - a^{\mu_2}(1+\mu_2 \ln a) < 0,
\end{aligned} \tag{14}$$

where $\mu_1 \in (d_{v_q}, d_{v_q}+1), \mu_2 \in (d_{x_i}-1, d_{x_i}), \mu_2 > \mu_1$ and $a > 1$.

$\mathrm{SEI}_a(G') < \mathrm{SEI}_a(G)$ which contradicts our choice of G. □

Lemma 10. *If $G \in \mathbb{U}_l(2m,m)$, $a > 1$ with maximum $SEI_a(G)$; then, for every vertex $x_i \in B$, there exist $T(x_i)$ which will be isomorphic to $\mathbb{T}^0(n_i, n_i/2)$ or $\mathbb{T}^0(n_i, n_i - 1/2)$. If $T(x_i)$ is isomorphic to $\mathbb{T}^0(n_i, n_i/2)$, then $d_{x_i} - 2$ will be equal to $\Delta(\mathbb{T}^0(n_i, n_i/2))$. If $T(x_i)$ is isomorphic to $\mathbb{T}^0(n_i, n_i - 1/2)$, then the vertex x_i will be the one end vertex of $\mathbb{T}^0(n_i, n_i - 1/2)$ and (x_i) will be adjacent to some maximum degree vertex of $\mathbb{T}^0(n_i, n_i - 1/2)$.*

Proof. Let $G \in \mathbb{U}_l(2m,m)$ with maximum variable sum exdeg index. We also assume that $x_i \in B$ and the vertices x_{i-1} and x_{i+1} are the neighbouring vertices of the vertex x_i along C_l. Here we consider the expression

$$\begin{aligned}
Q &= \left[d_{x_i}a^{d_{x_i}} - \left(d_{x_i}-2\right)a^{d_{x_i}-2}\right] + \left[d_{x_{i-1}}a^{d_{x_{i-1}}} - \left(d_{x_{i-1}}-1\right)a^{d_{x_{i-1}}-1}\right]\\
&\quad + \left[d_{x_{i+1}}a^{d_{x_{i+1}}} - \left(d_{x_{i+1}}-1\right)a^{d_{x_{i+1}}-1}\right].
\end{aligned} \tag{15}$$

We assume that G^* is the connected component of $G - \{x_i x_{i-1}, x_i x_{i+1}\}$ which does not contain the vertex x_i. We can write the expression $\mathrm{SEI}_a(G) = \mathrm{SEI}_a(G^*) + Q + \mathrm{SEI}_a(T(x_i))$.

According to Theorem 1, Lemma 7, and Lemma 8, we have

$$\mathrm{SEI}_a(G) \le \mathrm{SEI}_a(G^*) + Q + \mathrm{SEI}_a\left(\mathbb{T}^0\left(n_i, \frac{n_i}{2}\right)\right), \tag{16}$$

or

$$\mathrm{SEI}_a(G) \le \mathrm{SEI}_a(G^*) + Q + \mathrm{SEI}_a\left(\mathbb{T}^0\left(n_i, \frac{n_i - 1}{2}\right)\right), \tag{17}$$

for n_i being even or odd, respectively. Above two inequalities hold iff $T(x_i) \cong \mathbb{T}^0(n_i, n_i/2)$ and $T(x_i) \cong \mathbb{T}^0(n_i, n_i - 1/2)$, respectively. Next we will prove that

(1) If $T(x_i) \cong \mathbb{T}^0(n_i, n_i/2)$, then $d_{x_i} - 2 = \Delta(\mathbb{T}^0(n_i, n_i/2))$.
(2) If $T(x_i) \cong \mathbb{T}^0(n_i, n_i - 1/2)$, then $(\mathbb{T}^0(n_i, n_i - 1/2))$ has the vertex x_i as a pendent vertex that is adjacent to the vertex of maximum degree in $\mathbb{T}^0(n_i, n_i - 1/2)$.

For the proof of (i), we assume that $d_{x_i} - 2 < \Delta(\mathbb{T}^0(n_i, n_i/2))$. Let $y \in V(T)$, i.e., $d_y = \Delta(\mathbb{T}^0(n_i, n_i/2))$. We define $G' = G - x_i x_{i-1} - x_i x_{i+1} + x_{i-1} y + x_{i+1} y$. By the definition of $\mathrm{SEI}_a(G)$,

$$\begin{aligned}\mathrm{SEI}_a(G) - \mathrm{SEI}_a(G') &= \left[d_{x_i} a^{d_{x_i}} + d_y a^{d_y}\right] \\ &\quad - \left[\left(d_{x_i} - 2\right) a^{d_{x_i} - 2} + \left(d_y + 2\right) a^{d_y + 2}\right] \\ &= \left[d_{x_i} a^{d_{x_i}} - \left(d_{x_i} - 2\right) a^{d_{x_i} - 2}\right] \\ &\quad - \left[\left(d_y + 2\right) a^{d_y + 2} - d_y a^{d_y}\right].\end{aligned} \tag{18}$$

If $d_{x_i} \ge d_y$, then

$$\begin{aligned}\mathrm{SEI}_a(G) - \mathrm{SEI}_a(G') &= \left[d_y a^{d_y} - \left(d_{x_i} - 2\right) a^{d_{x_i} - 2}\right] \\ &\quad - \left[\left(d_y + 2\right) a^{d_y + 2} - d_{x_i} a^{d_{x_i}}\right] \\ &= z.\left[a^{\mu_1}\left(1 + \mu_1 \ln a\right) - a^{\mu_2}\left(1 + \mu_2 \ln a\right)\right] < 0,\end{aligned} \tag{19}$$

where $\mu_1 \in (d_x - 2, d_y)$, $\mu_2 \in (d_{x_i}, d_y + 2)$, $\mu_2 > \mu_1$, $a > 1$, and $z = d_y - d_{x_i} + 2$.

$\mathrm{SEI}_a(G') > \mathrm{SEI}_a(G)$ which contradicts our choice of G.

If $d_{x_i} < d_y$, then

$$\begin{aligned}\mathrm{SEI}_a(G) - \mathrm{SEI}_a(G') &= \left[d_{x_i} a^{d_{x_i}} - \left(d_{x_i} - 2\right) a^{d_{x_i} - 2}\right] \\ &\quad - \left[\left(d_y + 2\right) a^{d_y + 2} - \left(d_y\right) a^{d_y}\right] \\ &= 2.\left[a^{\mu_1}\left(1 + \mu_1 \ln a\right) - a^{\mu_2}\left(1 + \mu_2 \ln a\right)\right] < 0,\end{aligned} \tag{20}$$

where $\mu_1 \in (d_{x_i} - 2, d_{x_i})$, $\mu_2 \in (d_y, d_y + 2)$, $\mu_2 > \mu_1$, and $a > 1$.

$\mathrm{SEI}_a(G') > \mathrm{SEI}_a(G)$ which contradicts our choice of G.

For the proof of (ii), we will just show that $d_{x_i} = 3$ and $d_{w_1} = \Delta(T(v_i))$ where $w_1 = N(x_i) - \{x_{i+1}, x_{i-1}\}$.

Since $G \in \mathbb{U}_l(2m, m)$ and $T(x_i)$ is isomorphic to $\mathbb{T}^0(n_i, n_i - 1/2)$, $d_{x_i} - 2 < \Delta(\mathbb{T}^0(n_i, n_i - 1/2))$.

Note that any vertex w_2 other than the vertex of maximum degree in $\mathbb{T}^0(n_i, n_i - 1/2)$ has the degree 2 or 1. If $d_{x_i} - 2 = 2$, this implies that in $\mathbb{T}^0(n_i, n_i - 1/2)$, there will be a vertex which is not saturated by the maximal matching of G. Here a contradiction arises for $d_{x_i} - 2 = 1$. This implies $d_{x_i} = 3$. If we assume $d_{w_1} < \Delta(\mathbb{T}^0(n_i, n_i - 1/2))$, then once again we find a vertex in $\mathbb{T}^0(n_i, n_i - 1/2)$ which is not saturated by the maximal matching in G and again we will find a contradiction. From the above discussion, the proof is accomplished. □

Theorem 3. *Suppose $G \in \mathbb{U}_l(2m, m)$; then, $SEI_a \ge 1 + 3a^3 + 2(2m - 2)a^2$ for $a > 1$ and the sign of equality meets when $G \cong (C_l, x_i) \Cup (P_{2m-k+1}, x_i)$ where $x_i \in C_l$ is a pendent vertex of P_{2m-k+1}.*

Proof. Suppose $G \in \mathbb{U}_l(2m, m)$ having minimum SEI_a. According to Lemma 9, for the minimum $\mathrm{SEI}_a(G)$, $T(x_{s_t})$ will be isomorphic to $P_{n_{s_t}}$ for every $x_{s_t} \in B$ where $n_{s_t} = n(T(x_{s_t}))$. For $|B| = 1$, the above result holds. Now we discuss the above result for $|B| \ge 2$. We have $T(x_{s_t}) \cong P_{n_{s_t}}$ $(t = 1, 2, \ldots, |B|)$. So, we denote $T(x_{s_t}) = y_0^t y_1^t \ldots y_{b_t}^t$ $(b_t \ge 1)$, where $y_0^t = x_{s_t}$ $(t = 1, 2 \ldots .|B|)$. We define $G^* = G - y_0^2 \quad y_1^2 - y_0^3 y_1^3 \ldots - y_0^{|B|} y_1^{|B|} + y_{b_1}^1 y_1^2 \quad + y_{b_2}^2 y_1^3 + \cdots + y_{b_{|B|-1}}^{|B|-1} y_1^{|B|}$. It is clear that $G^* \in \mathbb{U}_l(2m, m)$; then, by the definition of SEI_a,

$$\begin{aligned}\mathrm{SEI}_a(G^*) - \mathrm{SEI}_a(G) &= (|B| - 1)\left[\left(2a^2 - a\right) - \left(3a^3 - 2a^2\right)\right] \\ &= (|B| - 1)\left[a^{\mu_1}\left(1 + \mu_1 \ln a\right) - a^{\mu_2}\left(1 + \mu_2 \ln a\right)\right] < 0,\end{aligned} \tag{21}$$

where $\mu_1 \in (1, 2)$, $\mu_2 \in (2, 3)$, $\mu_2 > \mu_1$, and $a > 1$.

$\mathrm{SEI}_a(G^*) < \mathrm{SEI}_a(G)$ which contradicts our choice of G. Hence, the proof of above theorem is finished. □

5. Main Result

Theorem 4. *Let $G \in \mathbb{U}_l(2m, m)$ and $a > 1$; then, the following results must hold:*

(1) If $2m = l + 2$, then $SEI_a \le 2a + 2(l - 2)a^2 + 3a^3$ and the sign of equality meets when G is not isomorphic to (C_l, P_3).
(2) If $2m \ge l + 3$ and l is odd, then $SEI_a(G) \le (m - l - 1/2)a + 2(m + l - 3/2)a^2 + (m - l - 5/2)a^{m-l-5/2}$ sign of equality meets iff $G \cong (C_l, x_i) \Cup (\mathbb{T}^0(2m - l + 1, 2m - l + 1/2), x_i)$.
(3) If $2m \ge l + 3$ and l is even, then $SEI_a(G) \le (m - l/2)a + 2(m + l/2 - 2)a^2 + 3a^3 + (m - l/2 + 1)a^{m-l/2+1}$ sign of equality meets iff $G \cong (C_l, x_i) \Cup (\mathbb{T}^0(2m - l + 1, 2m - l/2), x_i)$, where $d_{x_i} = 3$, $N(x_i) - \{x_{i-1}, x_{i+1}\} = y$, and $y = \Delta(\mathbb{T}^0(2m - l + 1, 2m - l/2), x_i)$.

Proof. Let $G \in \mathbb{U}_l(2m, m)$, $a > 1$ with maximum $\mathrm{SEI}_a(G)$. According to Lemma 8, we are sure that $T(x_i)$ is isomorphic to $\mathbb{T}^0(n_i, n_i - 1/2)$ or $\mathbb{T}^0(n_i, n_i/2)$ where $x_i \in B$.

For $|B| = 1$, we have no graph $G \not\cong (C_l, P_3)$ for which $2m = l + 2$. Whenever $2m = l + 2$, then G must be isomorphic to (C_l, P_3) where $G \in \mathbb{U}_l(2m, m)$. According to Theorem 3, we can find a graph G' such that $\mathrm{SEI}_a(G') > \mathrm{SEI}_a(C_l, P_3) = \mathrm{SEI}_a(G)$ for $G' \neq (C_l, P_3)$ which contradicts the choice of G. With the help of Lemma 10, the proof of (2) or (3) is satisfied. For $|B| \geq 2$, we may have the below cases.

Case 1. Let $2m = l + 2$; then, for any two graphs G^* and G^{**}, both graphs are not isomorphic to (C_l, P_3) and $\mathrm{SEI}_a(G^*) = \mathrm{SEI}_a(G^{**})$. According to Theorem 3, we have $\mathrm{SEI}_a(G) > \mathrm{SEI}_a((C_l, P_3))$ where $G \not\cong (C_l, P_3)$, and hence (1) satisfies.

Case 2. For $2m \geq l + 3$, we make the following subcases. Let $x_{s_t} \in B, t = 1, 2, \ldots, |B|$ and $n(T(x_{s_t})) = n_t$.

Subcase 2.1. Let $n_t = 2$ for every $x_{s_t} \in B$; then, we have the following set of vertices: $V(G) - V(C_l) = \{y_1, y_2, \ldots, y_{|B|}\}$ and $N(y_t) = x_{s_t}$, $t = 1, 2, \ldots, |B|$. Let $N(x_{s_t}) - \{y_t\} = \{x_{s_t} - 1, x_{s_t} + 1\}$, $t = 1, 2, \ldots, |B|$. Choose $|B| \geq 3$. If $|B| = 3$, we define $G^* = G - x_{s_2}y_2 - x_{s_3}y_3 + x_{s_1}y_2 + y_2y_3$. If $|B| \geq 4$, we define $G^* = G - x_{s_2}y_2 - x_{s_3}y_3 - x_{s_2-1}x_{s_2} - x_{s_2}x_{s_2+1} - x_{s_3}x_{s_3+1} + x_{s_2-1}x_{s_2+1} + x_{s_2}x_{s_3} + x_{s_2}x_{s_3+1} + x_{s_1}y_2 + y_2y_3$

In both above G^*, we have $G^* \in \mathbb{U}_l(2m, m)$ and we have the expression

$$\begin{aligned}\mathrm{SEI}_a(G^*) - \mathrm{SEI}_a(G) &= \left(4a^4 - 3a^3\right) + \left(2a^2 - a\right) \\ &\quad - 2\left(3a^3 - 2a^2\right) = \left(4a^4 - 3.3a^3\right) \\ &\quad + \left(3.2a^2 - a\right) > 0,\end{aligned} \tag{22}$$

which contradicts our choice of G.

Subcase 2.2. Let $x_{s_{l'}} \in B$, i.e., $n_{l'} = 3$; here we have $|B| \geq 2$; there must exist a vertex $x_{s_{t'}}$ in $B - \{x_{s_{l'}}\}$. We define $G^* = G - x_{s_{l'}}y_{l'} + x_{s_{t'}}y_{l'}$; then, clearly $G^* \in \mathbb{U}_l(2m, m)$. By the definition of $\mathrm{SEI}_a(G)$, we have

$$\begin{aligned}\mathrm{SEI}_a(G^*) - \mathrm{SEI}_a(G) &= \left[\left(d_{xs_{t'}} + 1\right)a^{d_{xs_{t'}}+1} + 2a^2\right] \\ &\quad - \left[d_{xs_{t'}}a^{d_{xs_{t'}}} + 3a^3\right] \\ &= \left[\left(d_{xs_{t'}} + 1\right)a^{d_{xs_{t'}}+1} - \left(d_{xs_{t'}}a^{d_{xs_{t'}}}\right)\right] \\ &\quad - \left[3a^3 - 2a^2\right].\end{aligned} \tag{23}$$

Since $d_{xs_{t'}} \geq 3$ and $a > 1$, this implies that $\mathrm{SEI}_a(G^*) - \mathrm{SEI}_a(G) > 0$ which is a contradiction to the choice of G.

Subcase 2.3. Let $x_{s_t} \in B$ and $n_t \geq 4$. In this concern, two subcases arise.

Subcase 2.3.1. Suppose that $d_{x_{s_l}} = \Delta(G)$ for some $x_{s_l} \in B$; since we have $|B| \geq 2$, there exists a vertex x_{s_r} in $B - \{x_{s_l}\}$. According to Lemma 8, Lemma 3, and Lemma 5, there must exist some adjacent vertices say u_s and v_s in $T(x_{s_r})$, i.e., $d_{u_s} = 2$ and $d_{v_s} = 1$. Let $N(u_s) - \{v_s\} = \{w_s\}$. We define $G^* = G - w_s u_s + x_{s_l}u_s$; then, clearly $G^* \in \mathbb{U}_l(2m, m)$ and

$$\begin{aligned}\mathrm{SEI}_a(G^*) - \mathrm{SEI}_a(G) &= \left[\left(d_{x_{s_l}} + 1\right)a^{d_{x_{s_l}}+1} - \left(d_{w_s} - 1\right)a^{d_{w_s}-1}\right] - \left[d_{x_{s_l}}a^{d_{x_{s_l}}} + d_{w_s}a^{d_{w_s}}\right] \\ &= \left[\left(d_{x_{s_l}} + 1\right)a^{d_{x_{s_l}}+1} - d_{x_{s_l}}a^{d_{x_{s_l}}}\right] - \left[d_{w_s}a^{d_{w_s}} - \left(d_{w_s} - 1\right)a^{d_{w_s}-1}\right] \\ &= \left[a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)\right] > 0,\end{aligned} \tag{24}$$

where $\mu_1 \in (d_{w_s} - 1, d_{w_s}), \mu_2 \in (d_{x_{s_l}}, d_{x_{s_l}} + 1), \mu_2 > \mu_1$, and $a > 1$.

$\mathrm{SEI}_a(G^*) > \mathrm{SEI}_a(G)$ which contradicts our choice of G.

Subcase 2.3.2. Suppose that $d_{x_{s_l}} < \Delta(G)$ for some $x_{s_l} \in B$. Let y be a vertex in G with $d_y = \Delta(G)$, so this implies that $y \in T(x_{s_l})$ where l is a positive integer. Since we have $|B| \geq 2$, then there exists some vertex x_{s_r} in $B - \{x_{s_l}\}$. According to Lemma 8, Lemma 3, and Lemma 5, there must exist some adjacent vertices say u_s and v_s in $T(x_{s_r})$, i.e., $d_{u_s} = 2$ and $d_{v_s} = 1$. Let $N(u_s) - \{v_s\} = \{w_s\}$.

Remaining portion of the under discussion subcase is similar to subcase 2.3.1 and once again we find the contradiction. According to all above discussion and argument, we follow the desired result. □

Theorem 5. *Let $G \in \mathbb{U}_l(2m, m)$, $a > 1$, and $n(T(x_i)) \geq 3$ for every $x_i \in B$; then,*

(1) If $2m \geq l + 3$ and l is odd, then $SEI_a(G) \leq (m - l - 1/2)a + 2(m + l - 3/2)a^2 + (m - l - 5/2)a^{m-l-5/2}$ sign of equality meets iff $G \cong (C_l, x_i) \Cup (\mathbb{T}^0(2m - l + 1, 2m - l + 1/2), x_i)$.

(2) If $2m \geq l + 3$ and l is even, then $SEI_a(G) \leq (m - l/2)a + 2(m + l/2 - 2)a^2 + 3a^3 + (m - l/2 + 1)a^{m-l/2+1}$ sign of equality meets iff $G \cong (C_l, x_i) \Cup (\mathbb{T}^0(2m - l + 1, 2m - l + 1/2), x_i)$, where

$d_{x_i} = 3, \quad N(x_i) - \{x_{i-1}, x_{i+1}\} = y, \quad$ *and* $y = \Delta(\mathbb{T}^0(2m - l + 1, 2m - l/2), x_i)$.

6. Extremal Values of Variable Sum Exdeg Index for Bicyclic Graphs

Here we are going to define some notations. Let $\mathbb{G}(n, n+1)$ be the collection of bicyclic graphs or all those graphs which have n vertices and $n+1$ number of edges. Note that if $G \in \mathbb{G}(n, n+1)$, then there exist two cycles say C_i and C_j in G.

(i) $\mathbb{A}(i, j)$ is the collection of graphs $G \in \mathbb{G}(n, n+1)$ in which cycles C_i and C_j share a single vertex only.

(ii) $\mathbb{B}(i, j)$ is the collection of graphs $G \in \mathbb{G}(n, n+1)$ in which cycles C_i and C_j share no common vertex.

(iii) $\mathbb{C}(i, j, l)$ is the collection of graphs $G \in \mathbb{G}(n, n+1)$ in which cycles C_i and C_j share a common path of length l.

6.1. Extremal Graphs in $\mathbb{A}(\mathbf{i}, \mathbf{j})$. Suppose $\mathbb{S}_n(i, j)$ is a graph from the collection $\mathbb{A}(i, j)$, i.e., there are $k = n - i - j + 1$ pendent vertices adjacent to a common vertex of C_i and C_j as shown in Figure 3.

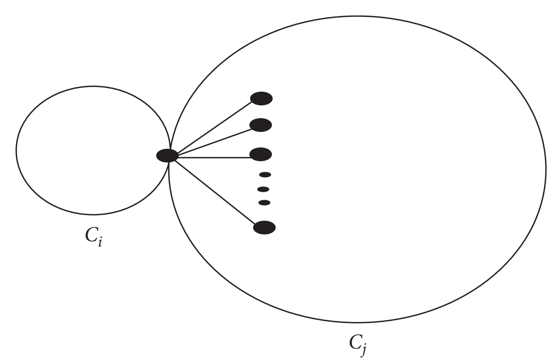

FIGURE 3: S_n *(i, j)* graphs.

Lemma 11. *Let* $G \in \mathbb{A}(i, j)$; *if* $G \not\cong \mathbb{S}_n(i, j)$, *then* $SEI_a(G) < SEI_a(\mathbb{S}_n(i, j))$ *for* $a > 1$.

Proof. Let $G \in \mathbb{A}(i, j)$; then, by Lemma 2, we obtain another graph say G' for which $\mathrm{SEI}_a(G') > \mathrm{SEI}_a(G)$. Further by Lemma 1, the graph G' can be changed into another graph say G'' in which pendent vertices will be attached with some common vertex u, of C_i and C_j. If u is a not a common vertex of C_i and C_j, then $G'' \not\cong \mathbb{S}_n(i, j)$. By the definition of $\mathrm{SEI}_a(G)$, we have

$$\begin{aligned}\mathrm{SEI}_a(\mathbb{S}_n(i, j)) - \mathrm{SEI}_a(G'') = &\left[(k+4).a^{k+4} + 2a^2\right] \\ &- \left[(k+2).a^{k+2} + 4a^4\right].\end{aligned} \tag{25}$$

Case − 1: for $k = n + 1 - i - j = 1$, $a > 1$, we have

$$\begin{aligned}\mathrm{SEI}_a(\mathbb{S}_n(i, j)) - \mathrm{SEI}_a(G'') &= \left[(k+4).a^{k+4} - 4a^4\right] - \left[(k+2).a^{k+2} - 2a^2\right] \\ &= \left[a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)\right] > 0,\end{aligned} \tag{26}$$

where $\mu_1 \in (2, k+2), \mu_2 \in (4, k+4), \mu_2 > \mu_1$, $a > 1$.

Case − 2: for $k = n + 1 - i - j \geq 2$, $a > 1$, we have

$$\begin{aligned}\mathrm{SEI}_a(\mathbb{S}_n(i, j)) - \mathrm{SEI}_a(G'') &= \left[(k+4).a^{k+4} - (k+2).a^{k+2}\right] - \left[4a^4 - 2a^2\right] \\ &= k.\left[a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)\right] > 0,\end{aligned} \tag{27}$$

where $\mu_1 \in (2, 4), \mu_2 \in (k+2, k+4), \mu_2 > \mu_1$, $a > 1$.

From the above two cases, we conclude that $\mathrm{SEI}_a(\mathbb{S}_n(i, j)) > \mathrm{SEI}_a(G'')$. □

Lemma 12. *Let* $\mathbb{S}_n(i, j) \in \mathbb{A}(i, j)$; *then,*

(a) $SEI_a(\mathbb{S}_n(i, j)) < SEI_a(\mathbb{S}_n(i-1, j))$, $a > 1$, $i > 3$.

(b) $SEI_a(\mathbb{S}_n(i, j)) < SEI_a(\mathbb{S}_n(i, j-1))$, $a > 1$, $j > 3$.

Proof. By the definition of $\mathrm{SEI}_a(G)$, we have

$$\begin{aligned}\mathrm{SEI}_a(\mathbb{S}_n(i, j)) - \mathrm{SEI}_a(\mathbb{S}_n(i-1, j)) &= \left[2a^2 - a\right] - \left[(k+5)a^{k+5} - (k+4)a^{k+4}\right] \\ &= a^{\mu_1}(1 + \mu_1 \ln a) - a^{\mu_2}(1 + \mu_2 \ln a) < 0,\end{aligned} \tag{28}$$

where $\mu_1 \in (1, 2), \mu_2 \in (k+4, k+5), \mu_2 > \mu_1$ and $a > 1\mathrm{SEI}_a(G') > \mathrm{SEI}_a(G)$.

Proof of (ii) is the same as proof of (i). □

Theorem 6. *If* $G \in \mathbb{A}(i, j)$, *then* $SEI_a(G)$ *will be maximal if* $G \cong \mathbb{S}_n(i, j)$ *and for all* $i \geq 3$, $j \geq 3$, *the graph from* $\mathbb{A}(i, j)$ *with maximum* SEI_a *is* $\mathbb{S}_n(3, 3)$.

Proof. Proof of this theorem can be obtained by Lemma 11 and Lemma 12. □

6.2. Extremal Graphs in $\mathbb{B}(\mathbf{i}, \mathbf{j})$. Here we define that $\mathbb{T}_n^r(i, j)$ is a graph which is obtained by joining C_i and C_j by a path P of length r and the remaining number of vertices $k = n - i - j - r + 1$ are attached to the same end vertex of P as shown in Figure 4.

Lemma 13. *Let* $G \in \mathbb{B}(i, j)$; *if* $G \not\cong \mathbb{T}_n^r(i, j)$, *then* $SEI_a(G) < SEI_a(\mathbb{T}_n^r(i, j))$ *for* $a > 1$.

Proof. Let $G \in \mathbb{B}(i, j)$; then, by Lemma 2, we obtain another graph say G' for which $\mathrm{SEI}_a(G') > \mathrm{SEI}_a(G)$. Further by

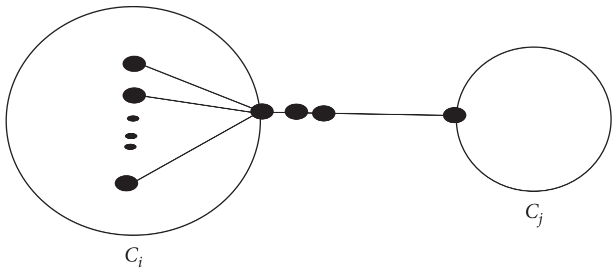

Figure 4: $\mathscr{T}_r\,(i,\,j)$ graphs.

Lemma 1, the graph G' can be changed into another graph say G'' in which pendent edges are attached with same vertex u, i.e., $\mathrm{SEI}_a(G'') > \mathrm{SEI}_a(G')$. If u is not end vertex of path P, then we will show $\mathrm{SEI}_a(\mathbb{T}_n^r) > \mathrm{SEI}_a(G'')$. By the definition of SEI_a, we have

$$\begin{aligned}\mathrm{SEI}_a(\mathbb{T}_n^r) - \mathrm{SEI}_a(G'') &= \left[(k+3)a^{k+3} - (k+2)a^{k+2}\right] - \left[3a^3 - 2a^2\right] \\ &= a^{\mu_2}(1+\mu_2 \ln a) - a^{\mu_1}(1+\mu_1 \ln a) > 0,\end{aligned} \tag{29}$$

where $\mu_1 \in (2,3), \mu_2 \in (k+2, k+3), \mu_2 > \mu_1$, $a > 1$, and $k = n+1-i-j-r$. □

Lemma 14. *Let $\mathbb{T}_n^r \in \mathbb{B}(\mathbf{i},\mathbf{j})$; then,*

(a) *$SEI_a(\mathbb{T}_n^r(i-1,j)) > SEI_a(\mathbb{T}_n^r(i,j))$, $a>1$, $i>3$.*
(b) *$SEI_a(\mathbb{T}_n^r(i,j-1)) > SEI_a(\mathbb{T}_n^r(i,j))$, $a>1$, $j>3$.*
(c) *$SEI_a(\mathbb{T}_n^{r-1}(i,j)) > SEI_a(\mathbb{T}_n^r(i,j))$, $a>1$, $r>1$.*

Proof. By the definition of $\mathrm{SEI}_a(G)$,

$$\begin{aligned}\theta &= \mathrm{SEI}_a(\mathbb{T}_n^r(i-1,j)) - \mathrm{SEI}_a(\mathbb{T}_n^r(i,j)) \\ &= \left[(k+4)a^{k+4} - (k+3)a^{k+3}\right] - \left[2a^2 - a\right] \\ &= a^{\mu_2}(1+\mu_2 \ln a) - a^{\mu_1}(1+\mu_1 \ln a) > 0,\end{aligned} \tag{30}$$

where $\mu_1 \in (1,2), \mu_2 \in (k+3,k+4), \mu_2 > \mu_1$, $a>1$, and $k = n+1-i-j-r$. This implies that $\theta > 0$.

Proof of (ii) is the same as proof of (i). □

Proof. By the definition of $\mathrm{SEI}_a(G)$,

$$\begin{aligned}\theta &= \mathrm{SEI}_a\left(\mathbb{T}_n^{r-1}(i,j)\right) - \mathrm{SEI}_a(\mathbb{T}_n^r(i,j)) \\ &= \left[(k+4)a^{k+4} - (k+3)a^{k+3}\right] - \left[2a^2 - a\right] \\ &= a^{\mu_2}(1+\mu_2 \ln a) - a^{\mu_1}(1+\mu_1 \ln a) > 0,\end{aligned} \tag{31}$$

where $\mu_1 \in (1,2), \mu_2 \in (k+3,k+4), \mu_2 > \mu_1$, $a>1$. This implies that $\theta > 0$.

$\mathrm{SEI}_a(\mathbb{T}_n^{r-1}(i,j)) > \mathrm{SEI}_a(\mathbb{T}_n^r(i,j))$. After proving Lemma 13 and Lemma 14, we are able to present the following theorem. □

Theorem 7. *If $G \in \mathbb{B}(i,j)$, then $SEI_a(G)$ will be maximal if $G \cong \mathbb{T}_n(i,j)$ and for all $i \geq 3$, $j \geq 3$, the graph from $\mathbb{B}(i,j)$ with maximum SEI_a is $\mathbb{T}_n(3,3)$.*

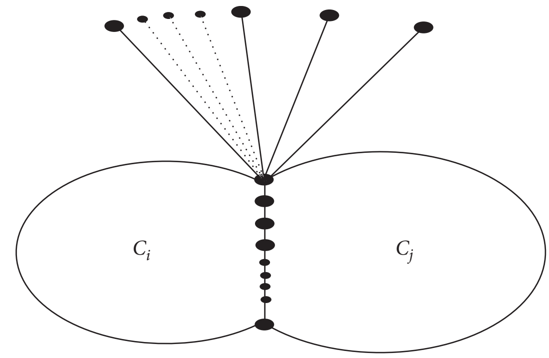

Figure 5: $\Lambda_n^l\,(i,\,j)$ graphs.

6.3. Extremal Graphs in $\mathbb{C}(\mathbf{i},\mathbf{j},\mathbf{l})$. Here we define that $\Lambda_n^l(i,j)$ is a graph which is obtained by attaching $n+l+1-i-j$ edges to one of the vertices of degree 3 in $G \in \mathbb{C}(i,j,l)$ (see Figure 5). Here we define some lemmas but skip their proofs. We refer Lemma 13 and Lemma 14 for the proof of following lemmas.

Lemma 15. *Let $G \in \mathbb{C}(i,j,l)$; if $G \ncong \Lambda_n^l(i,j)$, then $SEI_a(G) < SEI_a(\Lambda_n^l(i,j))$ for $a>1$.*

Lemma 16. *Let $\Lambda_n^l(i,j) \in \mathbb{C}(i,j,l)$; then,*

(a) *$SEI_a(\Lambda_n^l(i-1,j) > SEI_a(\Lambda_n^l(i,j))$, $i>3$.*
(b) *$SEI_a(\Lambda_n^l(i,j-1) > SEI_a(\Lambda_n^l(i,j))$, $j>3$.*
(c) *$SEI_a(\Lambda_n^{l-1}(i,j) > SEI_a(\Lambda_n^l(i,j))$, $l>1$.*

Theorem 8. *For $a>1$ and the graph from the collection $\mathbb{C}(i,j,l)$ with maximum $SEI_a(G)$ for all $i \geq 3$, $j \geq 3$ and $l > 1$ is $\Lambda_n^1(3,3)$.*

Theorem 9. *A graph $G \in \mathbb{G}(n,n+1)$ has maximum variable sum exdeg index if and only if $G \cong \Lambda_n^1(3,3)$ for $a>1$.*

Proof. Since $\mathbb{S}_n(3,3)$, $\mathbb{T}_n^1(3,3)$, and $\Lambda_n^1(3,3)$ belong to $\mathbb{G}(n,n+1)$. All the previous lemmas and theorems make it very clear and easy to understand that $\mathbb{S}_n(3,3)$, $\mathbb{T}_n^1(3,3)$, and $\Lambda_n^1(3,3)$ have maximum $\mathrm{SEI}_a(G)$, and $\mathbb{S}_n(3,3)$, $\mathbb{T}_n^1(3,3)$, and $\Lambda_n^1(3,3)$ belong to $\mathbb{A}(i,j)$, $\mathbb{B}(i,j)$, and $\mathbb{C}(i,j,l)$, respectively, for $n \geq 6$. Now we just need to compare the SEI_a of $\mathbb{S}_n(3,3)$, $\mathbb{T}_n^1(3,3)$, and $\Lambda_n^1(3,3)$.

$$\begin{aligned}\theta_1 &= \mathrm{SEI}_a\left(\Lambda_n^1(3,3)\right) - \mathrm{SEI}_a(\mathbb{S}_n(3,3)) \\ &= \left[(n-1).a^{n-1} + 3.a^3 + 2.2a^2 + (n-4)a\right] \\ &\quad - \left[(n-1).a^{n-1} + 4.2a^2 + (n-5)a\right] \\ &= 3a^3 - 2.2a^2 + (n-5)a > 0.\end{aligned} \tag{32}$$

This implies that $\theta_1 > 0$.

$$\begin{aligned}\theta_2 &= \mathrm{SEI}_a(\mathbb{S}_n(3,3)) - \mathrm{SEI}_a\left(\mathbb{T}_n^1(3,3)\right)\\ &= \left[(n-1).a^{n-1} + 4.2a^2 + (n-5)a\right]\\ &\quad - \left[(n-3).a^{n-3} + 4.2a^2 + 3.a^3 + (n-6)a\right]\\ &= \left[(n-1)a^{n-1} - (n-3)a^{n-3}\right] - \left[3a^3 - a\right]\\ &= 2\left[a^{\mu_2}(1+\mu_2 \ln a) - a^{\mu_1}(1+\mu_1 \ln a)\right] > 0,\end{aligned} \tag{33}$$

where $\mu_1 \in (1,3), \mu_2 \in (n-3, n-1), \mu_2 > \mu_1, a > 1$. This implies that $\theta_2 > 0$. From the above discussion, we conclude that $\Lambda_n^1(3,3) > \mathbb{S}_n(3,3) > \mathbb{T}_n^1(3,3)$. □

7. Conclusion

Ascertaining the upper and lower bounds on any molecular structure descriptor with regard to various graph parameters is a significant job. We have sought the maximum value of SEI_a for unicyclic graphs. Sharp bounds have also been investigated for conjugated trees and conjugated unicyclic graphs. We also investigated the extremal graphs for each upper and lower bounds. Following are the main points of conclusion.

(i) We have provided maximum and minimum values of SEI_a for conjugated trees.

(ii) We have also provided lower and upper bounds of SEI_a for unicyclic conjugated graphs with respect to the length of this cycle.

(iii) At the end of this paper, we have determined the maximum value of SEI_a for bicyclic graphs or $(n, n+1)$ − graphs.

Data Availability

The data used to support the findings of this study are included within the article. However, the reader may contact the corresponding author for more details of the data.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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