symmetry MDPI

Article

Ordering Unicyclic Connected Graphs with Girth g ≥ 3 Having Greatest SK Indices

Wang Hui [1], Adnan Aslam [2], Salma Kanwal [3,*], Mahnoor Akram [3], Tahira Sumbal Shaikh [3] and Xuewu Zuo [1]

1 General Education Department, Anhui Xinhua University, Hefei 230088, China
2 Department of Natural Sciences and Humanities, University of Engineering and Technology, Lahore 54000, Pakistan
3 Department of Mathematics, Lahore College for Women University, Lahore 54000, Pakistan
* Correspondence: salma.kanwal@lcwu.edu.pk

Abstract: For a graph, the *SK* index is equal to the half of the sum of the degrees of the vertices, the SK_1 index is equal to the half of the product of the degrees of the vertices, and the SK_2 index is equal to the half of the square of the sum of the degrees of the vertices. This paper shows a simple and unified approach to the greatest *SK* indices for unicyclic graphs by using some transformations and characterizes these graphs with the first, second, and third *SK* indices having order $r \geq 5$ and girth $g \geq 3$, where girth is the length of the shortest cycle in a graph.

Keywords: *SK* indices; graph transformations; girth; pendant vertex; unicyclic graphs

Citation: Hui, W.; Aslam, A.; Kanwal, S.; Akram, M.; Shaikh, T.S.; Zuo, X. Ordering Unicyclic Connected Graphs with Girth g ≥ 3 Having Greatest SK Indices. *Symmetry* **2023**, *15*, 871. https://doi.org/10.3390/sym15040871

Academic Editor: Michel Planat

Received: 1 March 2023
Revised: 30 March 2023
Accepted: 1 April 2023
Published: 6 April 2023

1. Background Survey and Preliminary Results

In this paper, the term "graph" will always mean a simple, finite, and undirected graph. A graph [1] is an ordered pair $A = (V(A), E(A))$ which is a representation of vertex set $V(A)$ and edge set $E(A)$. Here, A is taken as a unicyclic connected graph having order r and size e. Let the degree of a vertex ω be denoted by $d_A(\omega)$ whereas the distance between two vertices ω and x be denoted by $d(\omega, x)$. If $d(\omega) = 1$ then ω is said to be a leaf or pendant vertex.

A graph invariant is a numerical parameter for the characterization of the topology of a graph which is calculated on the basis of a molecular graph of a chemical compound. Some invariants are degree based and some are based on distance.

For constructing relationships between the physical, chemical and biological characteristics and the arrangements of molecules in a chemical compound, the most useful tool is chemical invariants. These invariants are symmetric functions and provide us with a chance to examine or investigate the physical and chemical properties of molecules in a compound without the expenditure of money and time used in testing in a laboratory [2].

The most former topological index introduced by Harold Wiener is the Wiener index [3] which is expressed as

$$\mathrm{W}(A) = \sum_{\{\omega,x\}\subseteq V(A)} d_A(\omega, x) \tag{1}$$

i.e., the total of the distances between all of A's unordered vertex pairs. Gutman and Trinajstić [4] established the first degree-based topological indices, the Zagreb indices, more than 30 years ago. Balaban et al. named them the Zagreb group indices after 10 years. It was later reduced to the Zagreb index [5,6].

The first Zagreb index and second Zagreb indexare defined as

$$\mathrm{M}_1(A) = \sum_{\omega x\in E(A)} (d(\omega) + d(x)) = \sum_{\omega\in V(A)} (d(\omega))^2 \tag{2}$$

$$\mathrm{M}_2(A) = \sum_{\omega,x\in E(A)} (d(\omega)d(x)) \tag{3}$$

In 2016, Shigehalli and Kanabur [7] put forward the new degree-based graph invariants. These are presented as

$$\mathrm{SK}(A) = \sum_{\omega x \in E(A)} \frac{d(\omega) + d(x)}{2} \tag{4}$$

$$\mathrm{SK}_1(A) = \sum_{\omega x \in E(A)} \frac{d(\omega)d(x)}{2} \tag{5}$$

$$\mathrm{SK}_2(A) = \sum_{\omega x \in E(A)} [\frac{d(\omega) + d(x)}{2}]^2 \tag{6}$$

In the last 30 years, many researchers and scholars have been working on the chemical graph theory. Many authors worked on these connectivity indices.

Shigehalli et al. [7] computed SK indices of the H-naphtalenic nanotube and the $T \cup C_4[m,n]$ nanotube. In [8], Shigehalli et al. obtained the explicit formulas without the aid of a computer for the polyhex nanotube. In [9], SK indices first appeared and also their explicit formula for Graphene was obtained. In [10], Shin Min Kang et al. calculated SK and some other indices of Porphyrin, Zinc-Porphyrin, Propyl Ether Imine, and Poly Dendrimers and also plotted them using Maple software. In [11], Ranjini and Lokeshacalculated the SK Indices of a graph operator subdivision graph $S(G)$ and semi-total point graph $R(G)$ on certain important chemical structures like tetracenic nanotubes and tetracenicnanotori. In [12], the behaviors of SK, SK_1 and SK_2 indices were investigated under some graphoperations by Nurkahli and Buyukkose. In [13], Roy and Ghosh concluded that the ETA descriptors were sufficiently rich in chemical information to encode the structural features contributing to the toxicities and these indices might be used in combination with other topological and physicochemical descriptors for the development of predictive $QSAR$ models. Recently, Lokesha et al. [14] established the SK indices of carbon nanocones using a $Q(A)$ operator. In [15], thegeneralized prism network of SK indices was investigated. In [16], Harisha et al. calculated the SK indices of the semi-total point graph $R(G)$ and subdivision graph $S(G)$ on tetracenic nanotubes and tetracenicnanotori, two significant chemical structures. In [17], the behaviors of SK indices were investigated under some graph operations when defined on weighted and interval weighted graphs.

1.1. Some Graph Transformations

In 2014, Tomescu et al. [18] used first and defined other three graph transformations to find the minimum, second and third minimum general sum connectivity indices of unicyclic connected graphs having fixed order and girth. These transformations are listed below.

M_1-transformation: In general, let yz be an edge whose vertices y and z have no common neighbor in a connected graph, where $d(y), d(z) \geq 2$. Furthermore, let $M_1(A)$ be the graph obtained by deleting an edge yz, identifying y and z in a new vertex t and adding a pendant edge to it.

In particular, let there be a connected unicyclic graph A with two nearby vertices ω_i, ω_{i+1} having no common neighbor in A, such that μ and ν pendant edges are linked to ω_i and ω_{i+1} with $d(\omega_i) = \mu + 2$ and $d(\omega_{i+1}) = \nu + 2$, respectively, where $d(\omega_i, \omega_{i+1}) \geq 2$. Then, the graph obtained by contracting edge $\omega_i\omega_{i+1}$ and attaching a new pendant edge to vertex ω_i is $M_1(A)$. (See Figure 1).

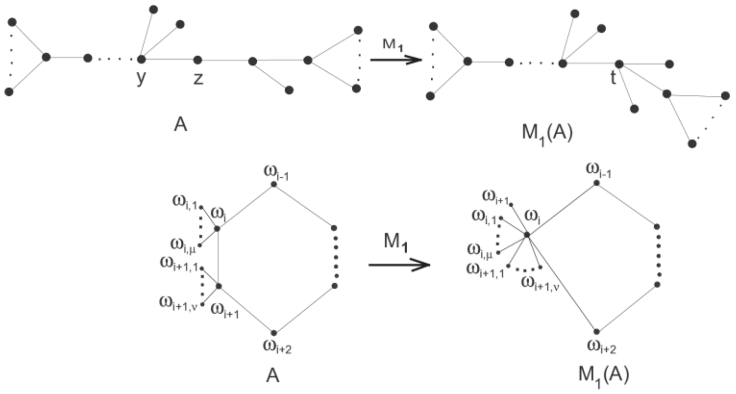

Figure 1. M_1-transformation.

M_2-transformation: Let ω_i, ω_{i+1} be the neighboring vertices with pendant edges such that $d(\omega_i) = \mu + 2$, $d(\omega_{i+1}) = \nu + 2$ in a connected unicyclic graph A where $\mu, \nu \geq 1$. Furthermore, after removing all the pendant edges incident to ω_i and attaching them to ω_{i+1}, we obtained a graph $M_2(A)$ (see Figure 2).

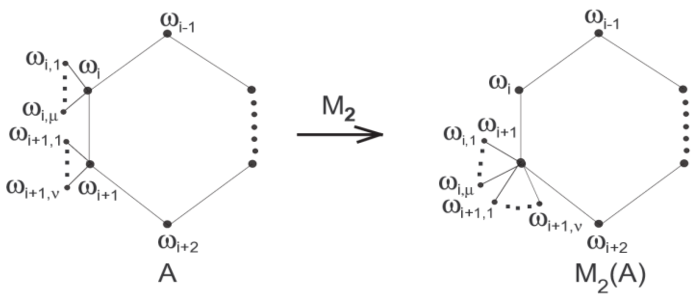

Figure 2. M_2-transformation.

M_3-transformation: Let A be a unicyclic graph with vertices ω_i, ω_j such that their distance $d(\omega_i, \omega_j) \geq 2$ where $d(\omega_i) = \mu + 2$, $d(\omega_j) = \nu + 2$; $1 \leq \mu \leq \nu$. Then, the graph we have after deleting one pendant edge from ω_i and adding it to ω_j is $M_3(A)$ (see Figure 3).

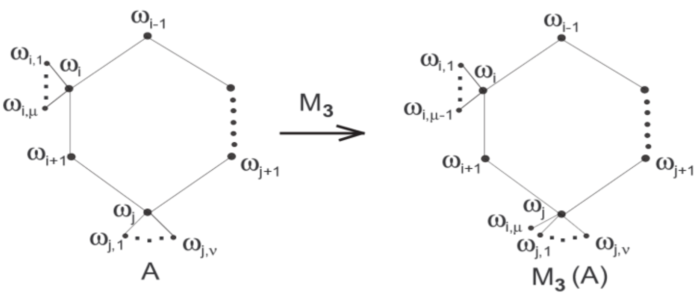

Figure 3. M_3-transformation.

M_4-transformation: Let ω_i, ω_{i+1} be neighboring vertices of a unicyclic connected graph A such that $d(\omega_i) = \mu + 2$, $d(\omega_{i+1}) = \nu + 2$; $1 \leq \mu \leq \nu$. By M_4-transformation, the graph $M_4(A)$ is attained by separating one pendant edge from ω_i and connecting it to ω_{i+1} (see Figure 4).

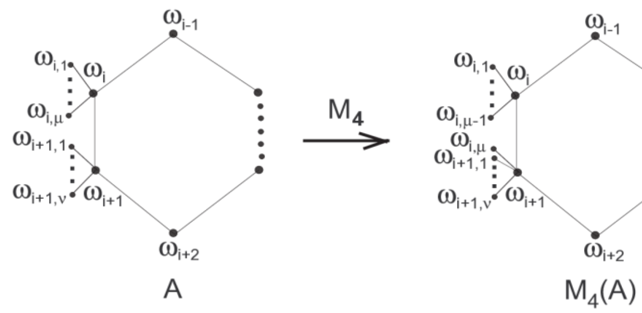

Figure 4. M_4-transformation.

1.2. Certain Unicyclic Graphic Structures

Let a unicyclic graph $U_r(\mu)$ which is deduced from $X(r-\mu, 3; r-\mu-3, 0, 0)$ by adding μ pendant edges to a pendant vertex of it, where $1 \leq \mu \leq r-4$.

Let the set of unlabelled connected unicyclic graphs be denoted by $O_{r,g}$ having order r and girth g where $r \geq g \geq 3$. A unicyclic graph $X(r, g; r_1, r_2, \ldots, r_g)$ with $r_i \geq 0$ is obtained by joining the r_i pendant edges to a vertex ω_i; $1 \leq i \leq g$ of cycle $C_g = \omega_1, \omega_2, \ldots, \omega_g, \omega_1$ where $r_1 + r_2 + \ldots + r_g = r - g$. Moreover, $X_{r,g} = X(r, g; r-g, 0, \ldots, 0)$ (see Figure 5).

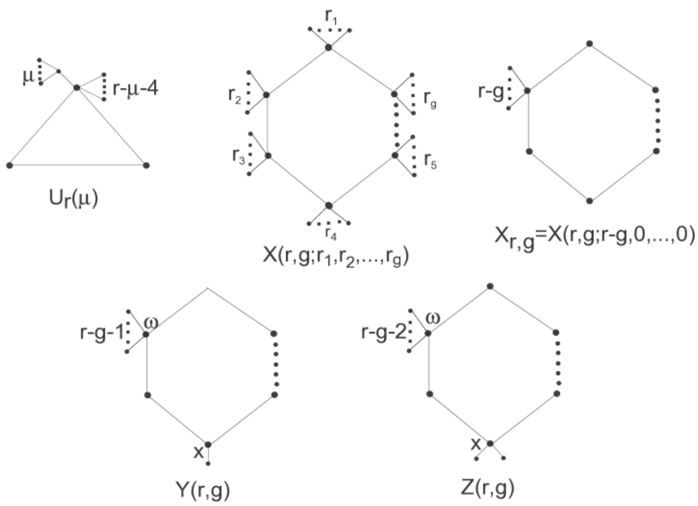

Figure 5. Some graph sets.

We will also use two sets of unicyclic connected graphs:

(i) $Y(r, g)$ is the family of unicyclic graphs in which the $r-g-1$ pendant edges are incident to a vertex $\omega \in V(C_g)$ and one pendant edge to $x \in V(C_g)$, where $d(\omega, x) \geq 2$.

(ii) $Z(r, g)$ is the set of unicyclic graphs in which the $r-g-2$ pendant edges are incident to ω and two pendant edges are incident to x, where $d(\omega, x) \geq 2$.

In $Y(r, g)$ and $Z(r, g)$, all graphs have similar index and properties. If $E \in Y_{r,g}$ and $F \in Z_{r,g}$ then $E = M_3(F)$. Moreover, we will utilize six different kinds of graphs to prove our main result, that are defined below:

(i) $A_1 = X(r, g; \mu-1, 1, 0, \ldots, 0)$ where $\mu = r-g \geq 2$.

(ii) $A_2 = X(r, g; \mu-2, 0, 2, 0, \ldots, 0)$ where $\mu = r-g \geq 2$. It can be easily seen that $A_2 \in Z_{r,g}$.

(iii) $A_3 = X(r, g; \mu-1, 0, 1, 0, \ldots, 0)$.

(iv) A_4: It is deduced by attaching one pendant edge to a pendant vertex of $X(r-1, g; \mu-1, 0, \ldots, 0)$

(v) A_5: It is obtained by connecting the $\mu-1$ pendant edges to the pendant vertex of $X(r-\mu+1, g; 1, 0, \ldots, 0)$.

(vi) $A_6 = X(r, g; \mu - 2, 2, 0, \ldots, 0)$.
(See Figure 6.)

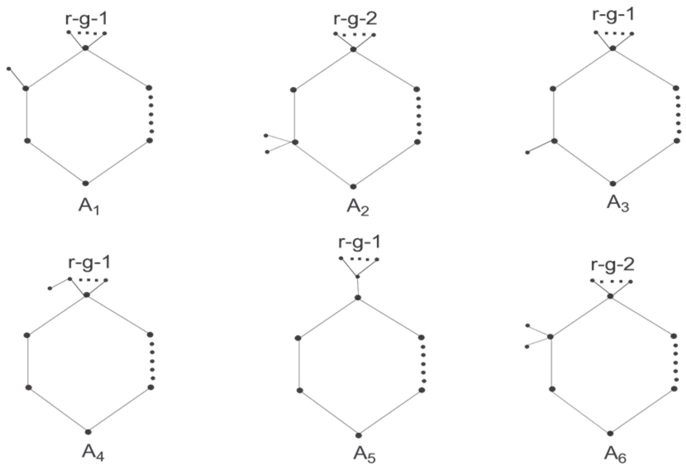

Figure 6. Some unicyclic graphs.

In this paper, we study three maximum SK indices, i.e., $SK(A)$, $SK_1(A)$ and $SK_2(A)$ in a unicyclic connected graph A having order $r \geq 5$ and girth $g \geq 3$.

2. Ordering Unicyclic Structures with the Greatest *SK* Index

In this section, we use some graph transformations which increase the SK index.

Lemma 1. *Let $M_1(A)$ be a unicyclic connected graph as shown in* Figure 1, *then*

$$SK(A) < SK(M_1(A))$$

for any $\mu, v \geq 0$.

Proof. Case 1: Ref. [19] When M_1 is performed excluding the vertices of C_g

$$\begin{aligned} SK(A) - SK(M_1(A)) &= \frac{1}{2} \sum_{xy \in E(A) \setminus \{yz\}} [(d_x + d_y) - (d_x + d_y + d_z - 1)] \\ &+ \frac{1}{2} \sum_{xz \in E(A) \setminus \{yz\}} [(d_x + d_z) - (d_x + d_y + d_z - 1)] < 0; \; as \; d_y \geq 2 \end{aligned}$$

Case 2: When M_1 is performed on the vertices of C_g

We have $d_A(\omega_i) = d_{M_1(A)}(\omega_i) - v - 1 < d_{M_1(A)}(\omega_i)$ and $d_{M_1(A)}(\omega_i) + d_{M_1(A)}(\omega_{i+1}) = \mu + v + 4$.

Therefore, for $j = 1, \mu = 1, 2, \ldots, \mu$, $k = 1, v = 1, 2, \ldots, v$ and by the definition of SK index, we find

$$\begin{aligned} SK(A) - SK(M_1(A)) &= \tfrac{1}{2}[\{d(\omega_{i-1}) + d(\omega_i)\} + \mu\{d(\omega_{i,j}) + d(\omega_i)\} + \{d(\omega_i) \\ &+ d(\omega_{i+1})\} + v\{d(\omega_{i+1,k}) + d(\omega_{i+1})\} + \{d(\omega_{i+1}) + d(\omega_{i+2})\}] \\ &= \tfrac{1}{2}[\{d(\omega_{i-1}) + d(\omega_i)\} + (\mu + \nu + 1)\{d(\omega_{i,l}) + d(\omega_i)\} \\ &\{d(\omega_i) + d(\omega_{i+2})\}] \\ &= -(\mu + \nu + \mu\nu + 1) < 0 \; for \; \mu, \nu \geq 0. \end{aligned}$$

$$\Rightarrow SK(A) < SK(M_1(A)) \; \square$$

Lemma 2. *Let $M_2(A)$ be a unicyclic connected graph as depicted in Figure 2, where $d_A(\omega_i, \omega_{i+1}) = 1$. Then*

$$SK(A) < SK(M_2(A))$$

for any $v \geq \mu \geq 1$.

Proof. Since $d_{M_2(A)}(\omega_i) = 2 < d_A(\omega_i) = \mu + 2$ and $d_A(\omega_{i+1}) = \nu + 2 < d_{M_2(A)}(\omega_{i+1}) = \nu + \mu + 2$.

$$
\begin{aligned}
SK(A) - SK(M_2(A)) \quad &= \tfrac{1}{2}[\{d(u_{i-1}) + d(u_i)\} + \sum_{j=1}^{\mu} \\
&\{d(\omega_{i,j}) + d(\omega_i)\} + \{d(\omega_i) + d(\omega_{i+1})\} \\
&+ \sum_{k=1}^{\nu} \{d(\omega_{i+1,k}) + d(\omega_{i+1})\} + \{d(\omega_{i+1}) + d(\omega_{i+2})\}] - \tfrac{1}{2}[\{d(\omega_{i-1}) \\
&+ d(\omega_i)\} + \{d(\omega_i) + d(\omega_{i+1})\} + (\mu + \nu)\{d(\omega_{i,j}) + d(\omega_{i+1})\} \\
&+ \{d(\omega_{i+1}) + d(\omega_{i+2})\}] \\
&= \tfrac{1}{2}[\{d(\omega_{i-1}) + d(\omega_i)\} + \mu\{d(\omega_{i,j}) + d(\omega_i)\} + \{d(\omega_i) + d(\omega_{i+1})\} \\
&+ \nu\{d(\omega_{i+1,k}) + d(\omega_{i+1})\} + \{d(\omega_{i+1}) + d(\omega_{i+2})\}] - \tfrac{1}{2}[\{d(\omega_{i-1}) \\
&+ d(\omega_i)\} + \{d(\omega_i) + d(\omega_{i+1})\} + (\mu + \nu)\{d(\omega_{i,j}) + d(\omega_{i+1})\} \\
&+ \{d(\omega_{i+1}) + d(\omega_{i+2})\}] \\
&= \tfrac{1}{2}\{(2 + \mu + 2) + \mu(1 + \mu + 2) + (\mu + 2 + \nu + 2) + \nu(1 + \nu + 2) \\
&+ (\nu + 2 + 2)\} - \tfrac{1}{2}\{(2 + 2) + (2 + \mu + \nu + 2) \\
&+ (\mu + \nu)(1 + \mu + \nu + 2) + (\mu + \nu + 2 + 2)\} \\
&= -\mu\nu < 0 \; for \; \nu \geq \mu \geq 1.
\end{aligned}
$$

$$\Rightarrow SK(A) < SK(M_2(A)) \; \square$$

Lemma 3. *Let $M_3(A)$ be a unicyclic connected graph as presented in Figure 3, where $d_A(\omega_i, \omega_{i+1}) = d_{M_3(A)}(\omega_i, \omega_{i+1}) \geq 2$. Then*

$$SK(A) < SK(M_3(A)); v \geq \mu \geq 1$$

Proof. Following the previous lemma and by the definition of $SK(A)$ we find

$$
\begin{aligned}
SK(A) - SK(M_3(A)) \quad &= \tfrac{1}{2}[\{d(\omega_{i-1}) + d(\omega_i)\} + \sum_{k=1}^{\mu} \{d(\omega_{i,j}) + d(\omega_i)\} + \{d(\omega_i) + d(\omega_{i+1})\} \\
&+ \{d(\omega_{i+1}) + d(\omega_j)\} + \sum_{l=1}^{\nu} \{d(\omega_{j,\nu}) + d(\omega_j)\} + \{d(\omega_j) + d(\omega_{j+1})\}] \\
&- \tfrac{1}{2}[\{d(\omega_{i-1}) + d(\omega_i)\} + \sum_{k=1}^{\mu-1} \{d(\omega_{i,\mu-1}) + d(\omega_i)\} + \{d(\omega_i) \\
&+ d(\omega_{i+1})\} + \{d(\omega_{i+1}) + d(\omega_j)\} + \sum_{l=1}^{\nu+1} \{d(\omega_{j,\nu}) + d(\omega_j)\} \\
&+ \{d(\omega_j) + d(\omega_{j+1})\}] \\
&= \tfrac{1}{2}[\{d(\omega_{i-1}) + d(\omega_i)\} + \mu\{d(\omega_{i,j}) + d(\omega_i)\} + \{d(\omega_i) + d(\omega_{i+1})\} \\
&+ \{d(\omega_{i+1}) + d(\omega_j)\} + \nu\{d(\omega_{j,\nu}) + d(\omega_j)\} + \{d(\omega_j) + d(\omega_{j+1})\}] \\
&- \tfrac{1}{2}[\{d(\omega_{i-1}) + d(\omega_i)\} + (\mu - 1)\{d(\omega_{i,\mu-1}) + d(\omega_i)\} + \{d(\omega_i) \\
&+ d(\omega_{i+1})\} + \{d(\omega_{i+1}) + d(\omega_j)\} + (\nu + 1)\{d(\omega_{j,\nu}) + d(\omega_j)\} \\
&+ \{d(\omega_j) + d(\omega_{j+1})\}] \\
&= \tfrac{1}{2}\{(2 + \mu + 2) + \mu(1 + \mu + 2) + (\mu + 2 + 2) + (2 + \nu + 2) \\
&+ \nu(1 + \nu + 2) + (\nu + 2 + 2)\} - \tfrac{1}{2}\{2 + \mu - 1 + 2 + (\mu - 1) \\
&(1 + \mu - 1 + 2) + (\mu - 1 + 2 + 2) + (2 + 1 + \nu + 2) \\
&+ (\nu + 1)(1 + \nu + 1 + 2) + (\nu + 1 + 2 + 2)\} \\
&= \mu - (\nu + 1) < 0 \; \nu \geq \mu \geq 1
\end{aligned}
$$

$$\Rightarrow SK(A) < SK(M_3(A)) \; \square$$

Hence, the proof is complete.

Lemma 4. *Let $M_4(A)$be the connected unicyclic graph as illustrated in Figure 4. For any $v \geq \mu \geq 1$, we have*

$$SK(A) < SK(M_4(A))$$

Proof. If $d_A(\omega_i, \omega_{i+1}) = 1$ then $d_{M_4(A)}(\omega_i) + d_{M_4(A)}(\omega_{i+1}) = \mu + 2 + \nu + 2 = d_A(\omega_i) + d_A(\omega_j)$ and by the definition of $SK(A)$, we have

$$\begin{aligned} SK(A) - SK(M_3(A)) &= \tfrac{1}{2}[\{d(\omega_{i-1}) + d(\omega_i)\} + \sum_{k=1}^{\mu} \{d(\omega_{i,j}) + d(\omega_i)\} + \{d(\omega_i) + d(\omega_{i+1})\} \\ &+ \{d(\omega_{i+1}) + d(\omega_j)\} + \sum_{l=1}^{\nu} \{d(\omega_{j,\nu}) + d(\omega_j)\} + \{d(\omega_j) + d(\omega_{j+1})\}] \\ &- \tfrac{1}{2}[\{d(\omega_{i-1}) + d(\omega_i)\} + \sum_{k=1}^{\mu-1} \{d(\omega_{i,\mu-1}) + d(\omega_i)\} + \{d(\omega_i) \\ &+ d(\omega_{i+1})\} + \{d(\omega_{i+1}) + d(\omega_j)\} + \sum_{l=1}^{\nu+1} \{d(\omega_{j,\nu}) + d(\omega_j)\} \\ &+ \{d(\omega_j) + d(\omega_{j+1})\}] \\ &= \tfrac{1}{2}[\{d(\omega_{i-1}) + d(\omega_i)\} + \mu\{d(\omega_{i,j}) + d(\omega_i)\} + \{d(\omega_i) + d(\omega_{i+1})\} \\ &+ \{d(\omega_{i+1}) + d(\omega_j)\} + \nu\{d(\omega_{j,\nu}) + d(\omega_j)\} + \{d(\omega_j) + d(\omega_{j+1})\}] \\ &- \tfrac{1}{2}[\{d(\omega_{i-1}) + d(\omega_i)\} + (\mu - 1)\{d(\omega_{i,\mu-1}) + d(\omega_i)\} + \{d(\omega_i) \\ &+ d(\omega_{i+1})\} + \{d(\omega_{i+1}) + d(\omega_j)\} + (\nu + 1)\{d(\omega_{j,\nu}) + d(\omega_j)\} \\ &+ \{d(\omega_j) + d(\omega_{j+1})\}] \\ &= \tfrac{1}{2}\{(2 + \mu + 2) + \mu(1 + \mu + 2) + (\mu + 2 + 2) + (2 + \nu + 2) \\ &+ \nu(1 + \nu + 2) + (\nu + 2 + 2)\} - \tfrac{1}{2}\{2 + \mu - 1 + 2 + (\mu - 1) \\ &(1 + \mu - 1 + 2) + (\mu - 1 + 2 + 2) + (2 + 1 + \nu + 2) \\ &+ (\nu + 1)(1 + \nu + 1 + 2) + (\nu + 1 + 2 + 2)\} \\ &= \mu - (\nu + 1) < 0 \; \nu \geq \mu \geq 1 \end{aligned}$$

$$\Rightarrow SK(A) < SK(M_4(A)) \; \square$$

Now, first we find the extremal graphs having the greatest value and then give an ordering of the unicyclic connected graphs in decreasing order for the SK index.

Theorem 1. *Ref. [19] Let $X(r, 3; a, b, c)$; $a + b + c = r - 3$; $a \geq b \geq c \geq 1$ be a set of unicyclic connected graphs with $r \geq 5$. Then, the first maximum and second maximum values of the SK index are attained by $X(r, 3; r - 3, 0, 0)$ and $X(r, 3; r - 4, 1, 0)$, respectively, i.e.,*

$$SK(X(r, 3; r - 4, 1, 0)) < SK(X(r, 3; r - 3, 0, 0))$$

(See Figure 7.)

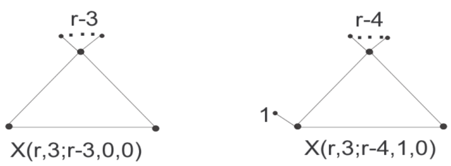

Figure 7. Unicyclic graphs having the first and second maximum SK index when $g = 3$.

Proof. We need only to prove $SK(X(r, 3; a, b, c)) < SK(X(r, 3; a + 1, b - 1, c))$. Consider

$$\begin{aligned}&SK(X(r,3;a,b,c)) - SK(X(r,3;a+1,b-1,c))\\&= \tfrac{1}{2}\{a(1+a+2) + (a+2+b+2) + b(1+b+2) + (b+2+c+2) + c(1+c+2)\\&+(c+2+a+2)\} - \tfrac{1}{2}\{(a+1)(1+a+1+2) + (a+1+2+b-1+2)\\&+(b-1)(1+b-1+2) + (b-1+2+c+2) + c(1+c+2) + (c+2+a+1+2)\}\\&= -a+b-1 < 0 \; for \; a \geq b \geq c \geq 1.\end{aligned}$$ □

Hence, the result follows.

Lemma 5. *Ref. [19] If $SK(U_r(\mu))$ is the maximum for fixed $r \geq 5$, where $1 \leq \mu \leq r-4$, then we have $\mu = 1$ or $r-4$.*

Proof. For $r = 5$, $\mu = 1 = r-4$ and there is only one graph $U_5(1)$. So, there cannot be a debate in choosing the maximum or minimum. Suppose that $3 \leq \mu \leq r-5$

$$\begin{aligned}SK(U_r(\mu)) &= \tfrac{1}{2}\{2(2+r-\mu-4+3) + (r-\mu-4)(1+r-\mu-4+3) + (r-\mu-4\\&+3+\mu+1) + \mu(1+\mu+1) + (2+2)\} = \tfrac{1}{2}(r^2+2\mu^2-r+4\mu-2r\mu+6)\end{aligned}$$

$$SK(U_r(\mu+1)) = \tfrac{1}{2}(r^2+2\mu^2+r+4\mu-2r\mu+10)$$

By using the above calculations, we determine

$$SK(U_r(\mu+1)) - SK(U_r(\mu)) = r+2 > 0$$

$$\Rightarrow SK(U_r(\mu+1)) > SK(U_r(\mu))$$

concluding that $SK(U_r(r-4)) > SK(U_r(\mu))$
where

$$SK(U_r(r-4)) = \frac{1}{2}(r^2-5r+22)$$

For $\mu = 1, 2$, we have

$$SK(U_r(1)) = \tfrac{1}{2}(r^2-3r+12)$$

$$SK(U_r(2)) = \tfrac{1}{2}(r^2-5r+22)$$

Furthermore

$$SK(U_r(1)) - SK(U_r(2)) = r-5 > 0$$

$$SK(U_r(1)) - SK(U_r(r-4)) = r-5 > 0$$

$$SK(U_r(2)) - SK(U_r(r-4)) = 0$$

By the above inequalities, we have

$$SK(U_r(1)) > SK(U_r(2)) = SK(U_r(r-4)) > SK(U_r(\mu)), U_r(\mu); 3 \leq \mu \leq r-5$$

The above used graphs are shown in Figure 8.

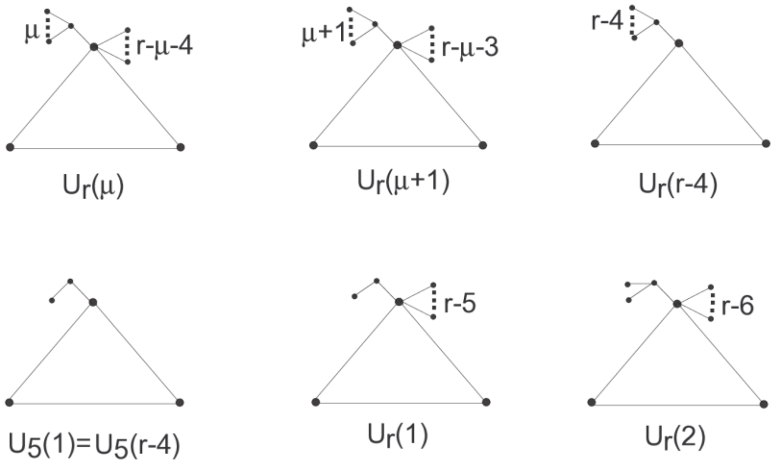

Figure 8. Graphs with the greatest SK index.

So, $U_r(1)$ is the graph with the first maximum and $U_r(2)$ and $U_r(r-4)$ with the second maximum SK index, and we are complete. □

Theorem 2. *Let A having girth g with $4 \leq g \leq r$, be a connected unicyclic graph. Then*

$$SK(A) \leq SK(X_{r,g})$$

where $X_{r,g} = X(r, g; r-g, 0, \ldots, 0)$.

Proof. Let $A \in O_{r,g}$, where $O_{r,g}$ be the set of unlabeled connected unicyclic graphs having order r and girth g with $r \geq g > 3$. If $g = r$, then $A = C_g$; for $g = r-1$ then $A = X(r, r-1; 1, 0, \ldots, 0)$. Suppose that $3 \leq g \leq r-2$ and A has the largest SK index. A is a graph with some vertex disjoint trees having each a common vertex with C_g. After applying M_1-transformation, the trees are reduced to some stars with centers on C_g and the SK index strictly increases by Lemma 1. Since $SK(A)$ is the maximum, it implies that $A = X(r, g; r_1, \ldots, r_g)$ where $r_1, \ldots, r_g \geq 0$ and $r_1 + \ldots + r_g = r - g$. All the pendant edges attached at the vertices of C_g are made incident to the unique and same vertex. After applying M_2, M_3-transformations several times, that would give $A = X_{r,g} = X(r, g; r-g, 0, \ldots, 0)$. □

Remark 1. *If $r-1 \geq g \geq 3$ then $SK(X(r, g; r-g, 0, \ldots, 0)) > SK(X(r, g+1; r-g-1, 0, \ldots, 0))$ by Case 1 of Lemma 1.*

Lemma 6. *For $p = r - g \geq 2$, we have*

(a) $SK(A_2) < SK(A_1)$
(b) $SK(A_3) = SK(A_1)$
(c) $SK(A_4) < SK(A_1)$
(d) $SK(A_5) < SK(A_1)$

(See Figure 8.)

Proof.

$$\begin{aligned}
&(a)\ SK(A_2) - SK(A_1) \\
&= \tfrac{1}{2}\{(2+\mu-2+2) + (\mu-2)(1+\mu-2+2) + (\mu-2+2+2) + (2+4) + (4+2) \\
&+(4+2)\} - \tfrac{1}{2}\{(2+\mu-1+2) + (\mu-1)(1+\mu-1+2) + (\mu-1+2+3) + (3+1) \\
&+(3+2) + (2+2)\} = -\mu + 1 < 0.
\end{aligned}$$

$(b)\ SK(A_3) - SK(A_1)$
$= \frac{1}{2}\{(\mu-1)(1+\mu-1+2) + (\mu-1+2+2) + (2+3) + (3+1) + (3+2)\}$
$-\frac{1}{2}\{(\mu-1)(1+\mu-1+2) + (\mu-1+2+3) + (3+1) + (3+2) + (2+2)\} = 0.$

$(c)\ SK(A_4) - SK(A_1)$
$= \frac{1}{2}\{(2+\mu-1+2) + (\mu-2)(1+\mu-2+3) + (\mu-2+3+2) + (2+1) + (\mu-1+2+2)$
$+(2+2)\} - \frac{1}{2}\{(2+\mu-1+2) + (\mu-1)(1+\mu-1+2) + (\mu-1+2+3) + (3+1)$
$+(3+2)\} = -1 < 0.$

$(d)\ SK(A_5) - SK(A_1)$
$= \frac{1}{2}\{(2+3) + (3+\mu-1+1) + (\mu-1)(1+\mu-1+1) + (3+2) + (2+2)\}$
$-\frac{1}{2}\{(2+\mu-1+2) + (\mu-1)(1+\mu-1+2) + (\mu-1+2+3) + (3+1) + (3+2)\}$ □
$= -\mu + 1 < 0.$

Theorem 3. *(a) Let* $A \in O_{r,g} \backslash \{X_{r,g}\}$*, where* $r \geq 6, (4 \leq g \leq r-2)$*. Then A has a maximum SK index if, and only if,* $A = A_1 (= A_3)$*.*
(b) Let $A \in O_{r,g} \backslash \{(A_1 \cup X_{r,g})\}$*, where* $r \geq 6, (4 \leq g \leq r-2)$*. Then A has a maximum SK index if, and only if,* $A = X(r, g; r-g-2, 0, 2, 0, \ldots, 0) = A_2$*.*

Proof. Let $A \in O_{r,g}$ be a connected unicyclic graph having the second or third maximum SK index. Suppose that there is a vertex with a degree of at least 3 in a cycle C_g of A. Since $A \neq X_{r,g}$, then there is at least one non-pendant vertex in C.

Case 1: When there is exactly one non-pendant vertex outside C, we obtained A by attaching the μ pendant edges to a pendant vertex of $X(r-\mu, g; r-g-\mu, 0, \ldots, 0)$ where $(1 \leq \mu \leq r-g-1)$. Lemma 5 states that for $\mu = 1$ or $r-4$ we have a maximum of $SK(U_r(\mu))$ with corresponding graphs A_4 and A_5, respectively.

However, Lemma 6 implies that the graphs with the second or third maximum SK index cannot be A_4 or A_5.

Case 2: When there are at least two non-pendant vertices outside C, after the continuous application of M_1-transformation, we have

$$SK(A) < max\{SK(A_4), SK(A_5)\} < SK(A_3) = SK(A_1) < SK(X_{r,g})$$

as $SK(A_1) - SK(X_{r,g}) = \{\frac{1}{2}(r^2+g^2+3r+g-2rg+2)\} - \{\frac{1}{2}(r^2+g^2+5r-g-2rg)\} = -r+g+1 < 0 \quad (7)$

Thus, we knew that if A has a second or third maximum SK index then the two vertices on C_g must exist having a degree of at least three.

(a) For $A \neq X_{r,g}$, if A has a maximum SK then C_g cannot have three vertices with a degree of at least 3.

We obtained $X_{r,g}$ after several applications of M_i-transformations $(i \geq 1)$. However, we found a graph with an index less than $X_{r,g}$, we see that

$$SK(A) < max\{SK(A_3), SK(A_1)\} = SK(A_3) = SK(A_1) < SK(X_{r,g})$$

It implies that A has exactly two vertices m, n on C_g having a degree of at least 3.

Degrees of m and n must be as: $d(m) = r-g+1, d(n) = 3$, since other cases cannot hold because if $d(m) = 2$ then A becomes $X_{r,g}$ (since our supposition of the degree is at least 3) and if $d(m) = 4$ then A cannot become the second maximum because A with $d(m) = 3$ has a greater index than A with $d(m) = 4$.

Now, if $d(m, n) = 1$ then $A = A_1$ and if $d(m, n) \geq 2$ then $A \in Y(r, g)$ class including A_3.

Lemma 6 implies that, in this case, extremal graph is A_1.

(b) For $A \in O_{r,g} \backslash (A_1 \cup X_{r,g})$, by the same argument we deduce that C_g cannot have three vertices with a degree of at least 3, if A has a maximum SK index, since, in this case, we would have

$$SK(A) < SK(A_2) < SK(A_3) = SK(A_1) < SK(X_{r,g})$$

$$\text{as } SK(A_2) - SK(A_1) = \left\{\frac{1}{2}\left(r^2 + g^2 + r + 3g - 2rg + 4\right)\right\} - \left\{\frac{1}{2}\left(r^2 + g^2 + 3r + g - 2rg + 2\right)\right\}$$
$$= \frac{1}{2}(-2r + 2g + 2) = -r + g + 1 < 0$$

It implies that A has exactly two vertices a, b on C_g having a degree of at least 3.

By the same argument (used above), $d(m) = r - g$ and $d(n) = 4$.

If $d(m,n) = 1$ then $A = A_6$ and if $d(m,n) \geq 2$ then $A \in Z(r,g)$ class including A_2, which ends the proof(see Figure 9). $\square$

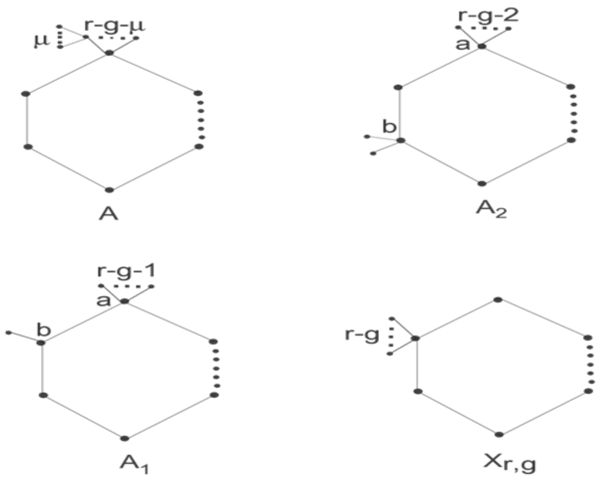

Figure 9. Unicyclic connected graphs having the greatest SK index.

3. Ordering Unicyclic Structures with the Greatest SK_1 Index

In this section, we use graph transformations which increase the SK_1 index.

Lemma 7. *Let $M_1(A)$ be a unicyclic connected graph as shown in Figure 1, then*

$$SK_1(A) < SK_1(M_1(A))$$

for any $\mu, v \geq 0$.

Proof. Case 1: Ref. [19] When M_1 is performed excluding vertices of C_g

$$\begin{aligned} SK_1(A) - SK_1(M_1(A)) &= \frac{1}{2} \sum_{xy \in E(A) \backslash \{yz\}} [(d_x.d_y) - (d_x)(d_y + d_z - 1)] \\ &+ \frac{1}{2} \sum_{xz \in E(A) \backslash \{yz\}} [(d_x.d_z) - (d_x)(d_y + d_z - 1)] < 0; \text{ as } d_y \geq 2 \end{aligned}$$

Case 2: When M_1 is performed on vertices of C_g

We have $d_A(\omega_i) = d_{M_1(A)}(\omega_i) - v - 1 < d_{M_1(A)}(\omega_i)$ and $d_{M_1(A)}(\omega_i) + d_{M_1(A)}(\omega_{i+1}) = \mu + v + 4$.

Therefore, for $j = 1, \mu = 1, 2, \ldots, \mu$, $k = \overline{1, v} = 1, 2, \ldots, v$ and by the definition of the SK_1 index, we find

$$\begin{aligned}
SK_1(A) - SK_1(M_1(A)) &= \tfrac{1}{2}[\{d(\omega_{i-1}).d(\omega_i)\} + \mu\{d(\omega_{i,j}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+1})\} \\
&+\nu\{d(\omega_{i+1,k}).d(\omega_{i+1})\} + \{d(\omega_{i+1}).d(\omega_{i+2})\}] - \tfrac{1}{2}[\{d(\omega_{i-1}).d(\omega_i)\} \\
&+(\mu+\nu+1)\{d(\omega_{i,j}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+2})\}] \\
&= \tfrac{1}{2}[\{(2)(\mu+2)\} + \mu\{(1)(\mu+2)\}\{(\mu+2)(\nu+2)\} \\
&+\nu\{(1)(\nu+2)\} + \{(\nu+2)(2)\}] - \tfrac{1}{2}[\{(2)(\mu+\nu+3)\} \\
&+(\mu+\nu+1)\{(1)(\mu+\nu+3)\} + \{(\mu+\nu+3)(2)\}] \\
&= -\{\mu+\nu+\tfrac{1}{2}(3+\mu\nu)\} < 0 \; for \; \mu,\nu \geq 1.
\end{aligned}$$

$$\Rightarrow SK_1(A) < SK_1(M_1(A)) \; \square$$

Lemma 8. *Let $M_2(A)$ be a unicyclic connected graph as depicted in Figure 2, where $d_A(\omega_i,\omega_{i+1}) = 1$. Then*

$$SK_1(A) < SK_1(M_2(A))$$

for any $v \geq \mu \geq 1$.

Proof. Since $d_{M_2(A)}(\omega_i) = 2 < d_A(\omega_i) = \mu + 2$ and $d_A(\omega_{i+1}) = \nu + 2 < d_{M_2(A)}(\omega_{i+1}) = \nu + \mu + 2$.

$$\begin{aligned}
SK_1(A) - SK_1(M_2(A)) &= \tfrac{1}{2}[\{d(\omega_{i-1}).d(\omega_i)\} + \sum_{j=1}^{\mu} \{d(\omega_{i,j}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+1})\} \\
&+\sum_{k=1}^{\nu} \{d(\omega_{i+1,k}).d(\omega_{i+1})\} + \{d(\omega_{i+1}).d(\omega_{i+2})\}] \\
&\tfrac{1}{2}[\{d(\omega_{i-1}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+1})\} + (\mu+\nu)\{d(\omega_{i,j}).d(\omega_{i+1})\} \\
&+\{d(\omega_{i+1}).d(\omega_{i+2})\}] \\
&= \tfrac{1}{2}[\{d(\omega_{i-1}).d(\omega_i)\} + \mu\{d(\omega_{i,j}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+1})\} \\
&+\nu\{d(\omega_{i+1,k}).d(\omega_{i+1})\} + \{d(\omega_{i+1}).d(\omega_{i+2})\}] \\
&\tfrac{1}{2}[\{d(\omega_{i-1}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+1})\} + (\mu+\nu)\{d(\omega_{i,j}).d(\omega_{i+1})\} \\
&+\{d(\omega_{i+1}).d(\omega_{i+2})\}] \\
&= \tfrac{1}{2}\{(2)(\mu+2) + \mu(1)(\mu+2) + (\mu+2)(\nu+2) + \nu(1)(\nu+2) \\
&+(\nu+2)(2)\} - \tfrac{1}{2}\{(2)(2) + (2)(\mu+\nu+2) + (\mu+\nu)(1)(\mu+\nu+2) \\
&+(\mu+\nu+2)(2)\} \\
&= -\tfrac{1}{2}(\mu\nu) < 0 \; for \; \nu \geq \mu \geq 1.
\end{aligned}$$

$$\Rightarrow SK_1(A) < SK_1(M_2(A)) \; \square$$

Lemma 9. *Let $M_3(A)$ be a unicyclic connected graph as presented in Figure 3, where $d_A(\omega_i,\omega_{i+1}) = d_{M_3(A)}(\omega_i,\omega_{i+1}) \geq 2$. Then*

$$SK_1(A) < SK_1(M_3(A)); v \geq \mu \geq 1$$

Proof. Following the previous lemma and by the definition of $SK_1(A)$, we find

$$\begin{aligned}
SK_1(A) - SK_1(M_3(A)) &= \tfrac{1}{2}[\{d(\omega_{i-1}).d(\omega_i)\} + \sum_{k=1}^{\mu} \{d(\omega_{i,j}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+1})\} \\
&+\{d(\omega_{i+1}).d(\omega_j)\} + \sum_{l=1}^{\nu} \{d(\omega_{j,\nu}).d(\omega_j)\} + \{d(\omega_j).d(\omega_{j+1})\}] \\
&-\tfrac{1}{2}[\{d(\omega_{i-1}).d(\omega_i)\} + \sum_{k=1}^{\mu-1} \{d(\omega_{i,\mu-1}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+1})\} \\
&+\{d(\omega_{i+1}).d(\omega_j)\} + \sum_{l=1}^{\nu+1} \{d(\omega_{j,\nu}).d(\omega_j)\} + \{d(\omega_j).d(\omega_{j+1})\}] \\
&= \tfrac{1}{2}[\{d(\omega_{i-1}).d(\omega_i)\} + \mu\{d(\omega_{i,j}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+1})\} \\
&+\{d(\omega_{i+1}).d(\omega_j)\} + \nu\{d(\omega_{j,\nu}).d(\omega_j)\} + \{d(\omega_j).d(\omega_{j+1})\}] \\
&-\tfrac{1}{2}[\{d(\omega_{i-1}).d(\omega_i)\} + (\mu-1)\{d(\omega_{i,\mu-1}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+1})\} \\
&+\{d(\omega_{i+1}).d(\omega_j)\} + (\nu+1)\{d(\omega_{j,\nu}).d(\omega_j)\} + \{d(\omega_j).d(\omega_{j+1})\}] \\
&= \tfrac{1}{2}\{(2)(\mu+2) + \mu(1)(\mu+2) + (\mu+2)(2) + (2)(\nu+2) \\
&+\nu(1)(\nu+2) + (\nu+2)(2)\} - \tfrac{1}{2}\{2(\mu-1+2) + (\mu-1)(1) \\
&(\mu-1+2) + (\mu-1+2)(2) + (2)(1+\nu+2) + (\nu+1)(1)(\nu+1+2) \\
&+(\nu+1+2)(2)\} \\
&= \tfrac{1}{2}(2\mu - 2\nu - 2) = \mu - \nu - 1 < 0 \ \nu \geq \mu \geq 1
\end{aligned}$$

$$\Rightarrow SK_1(A) < SK_1(M_3(A)) \ \square$$

Hence, the proof is complete.

Lemma 10. *Let $M_4(A)$ be the graph attained from A as illustrated in Figure 4. For any $\nu \geq \mu \geq 1$, we have*

$$SK_1(A) < SK_1(M_4(A))$$

Proof. If $d_A(\omega_i, \omega_{i+1}) = 1$ then $d_{M_4(A)}(\omega_i) + d_{M_4(A)}(\omega_{i+1}) = \mu + 2 + v + 2 = d_A(\omega_i) + d_A(\omega_j)$ and by the definition of $SK_1(A)$, we have

$$\begin{aligned}
SK_1(A) - SK_1(M_4(A)) &= \tfrac{1}{2}[\{d(\omega_{i-1}).d(\omega_i)\} + \sum_{j=1}^{\mu} \{d(\omega_{i,j}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+1})\} \\
&+\sum_{k=1}^{\nu} \{d(\omega_{i+1,k}).d(\omega_{i+1})\} + \{d(\omega_{i+1}).d(\omega_{i+2})\}] - \tfrac{1}{2}[\{d(\omega_{i-1}) \\
&.d(\omega_i)\} + \sum_{j=1}^{\mu-1} \{d(\omega_{i,\mu-1}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+1})\} \\
&+\sum_{k=1}^{\nu+1} \{d(\omega_{i+1,k}).d(\omega_{i+1})\} + \{d(\omega_{i+1}).d(\omega_{i+2})\}] \\
&= \tfrac{1}{2}[\{d(\omega_{i-1}).d(\omega_i)\} + \mu\{d(\omega_{i,j}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+1})\} \\
&+\nu\{d(\omega_{i+1,k}).d(\omega_{i+1})\} + \{d(\omega_{i+1}).d(\omega_{i+2})\}] - \tfrac{1}{2}[\{d(\omega_{i-1}) \\
&.d(\omega_i)\} + (\mu-1)\{d(\omega_{i,\mu-1}).d(\omega_i)\} + \{d(\omega_i).d(\omega_{i+1})\} \\
&+(\nu+1)\{d(\omega_{i+1,k}).d(\omega_{i+1})\} + \{d(\omega_{i+1}).d(\omega_{i+2})\}] \\
&= \tfrac{1}{2}\{(2)(\mu+2) + \mu(1)(\mu+2) + (\mu+2)(\nu+2) + \nu(1)(\nu+2) \\
&+(\nu+2)(2)\} - \tfrac{1}{2}\{(2)(\mu-1+2) + (\mu-1)(1)(\mu-1+2) \\
&+(\mu-1+2)(\nu+1+2) + (\nu+1)(1)(\nu+1+2) + (\nu+1+2)(2)\} \\
&= \tfrac{1}{2}(\mu - \nu - 1) < 0 \ for \ \nu \geq \mu \geq 1.
\end{aligned}$$

$$\Rightarrow SK_1(A) < SK_1(M_4(A)) \ \square$$

Now first, we find the extremal graphs having the greatest value and then give an ordering of the unicyclic connected graphs in decreasing order for the SK_1 index.

Theorem 4 (Ref. [19]). *Let $X(r,3;a,b,c); a+b+c=r-3; a \geq b \geq c \geq 1$ be a set of unicyclic connected graphs with $r \geq 5$. Then the first maximum and second maximum values of the SK_1 index are attained by $X(r,3;r-3,0,0)$ and $X(r,3;r-4,1,0)$, respectively, i.e.,*

$$SK_1(X(r,3;r-4,1,0)) < SK_1(X(r,3;r-3,0,0))$$

(See Figure 7.)

Proof. We need only to prove $SK_1(X(r,3;a,b,c)) < SK_1(X(r,3;a+1,b-1,c))$.

Consider

$$\begin{aligned}
&SK_1(X(r,3;a,b,c)) - SK_1(X(r,3;a+1,b-1,c))\\
&= \tfrac{1}{2}\{a(1)(a+2)+(a+2)(b+2)+b(1)(b+2)+(b+2)(c+2)+c(1)(c+2)\\
&+(c+2)(a+2)\} - \tfrac{1}{2}\{(a+1)(1)(a+1+2)+(a+1+2)(b-1+2)\\
&+(b-1)(1)(b-1+2)+(b-1+2)(c+2)+c(1)(c+2)+(c+2)(a+1+2)\}\\
&= \tfrac{1}{2}(-a+b-1) < 0 \; for \; a \geq b \geq c \geq 1.
\end{aligned}$$

Hence, the result follows. □

Lemma 11. (Ref. [19]). *If $SK_1(U_r(\mu))$ is the maximum for fixed $r \geq 5$, where $1 \leq \mu \leq r-4$, then we have $\mu = 1$* or $r-4$.

Proof. For $r=5$, $\mu = 1 = r-4$ and there is only one graph $U_5(1)$. So, there cannot be a debate in choosing the maximum or the minimum.

Suppose that $3 \leq \mu \leq r-5$

$$\begin{aligned}
SK_1(U_r(\mu)) \quad &= \tfrac{1}{2}\{2(2)(r-\mu-4+3)+(r-\mu-4)(1)(r-\mu-4+3)+(r-\mu-4+3)\\
&(\mu+1)+\mu(1)(\mu+1)+(2)(2)\} = \tfrac{1}{2}(r^2+\mu^2-r\mu+3)
\end{aligned}$$

$$SK_1(U_r(\mu+1)) = \tfrac{1}{2}(r^2+\mu^2+3r-r\mu+6)$$

By using the above calculations, we determine

$$SK_1(U_r(\mu+1)) - SK_1(U_r(\mu)) = \frac{3}{2}(r+1) > 0$$

$$\Rightarrow SK_1(U_r(\mu+1)) > SK_1(U_r(\mu))$$

concluding that $SK_1(U_r(\mu)) > SK_1(U_r(r-4))$

where

$$SK_1(U_r(r-4)) = \frac{1}{2}(r^2-4r+19)$$

For $p = 1,2$, we have

$$SK_1(U_r(1)) = \tfrac{1}{2}(r^2-r+4)$$

$$SK_1(U_r(2)) = \tfrac{1}{2}(r^2-2r+7)$$

Furthermore

$$SK_1(U_r(1)) - SK_1(U_r(2)) = \frac{1}{2}(r-3) > 0$$

$$SK_1(U_r(1)) - SK_1(U_r(r-4)) = \frac{3}{2}(r-5) > 0$$

$$SK_1(U_r(2)) - SK_1(U_r(r-4)) = r - 6 > 0$$

By the above inequalities, we have

$$SK_1(U_r(1)) > SK_1(U_r(2)) > SK_1(U_r(\mu)) > SK_1(U_r(r-4)), U_r(\mu); 3 \leq \mu \leq r-5$$

The above used graphs are shown in Figure 8. Therefore, $U_r(1)$ is a graph with the first maximum and $U_r(2)$ with the second maximum SK_1 index, and we are complete. □

Theorem 5. *Let A having girth g with $4 \leq g \leq r$, be a connected unicyclic graph. Then*

$$SK_1(A) \leq SK_1(X_{r,g})$$

where $X_{r,g} = X(r, g; r-g, 0, \ldots, 0)$.

Proof. Let $A \in O_{r,g}$, where $O_{r,g}$ be the set of unlabelled connected unicyclic graphs having order r and girth g with $r \geq g > 3$. If $g = r$, then $A = C_g$; for $g = r-1$ then $A = X(r, r-1; 1, 0, \ldots, 0)$. Suppose that $3 \leq g \leq r-2$ and A has the largest SK_1 index. A is a graph with some vertex disjoint trees having each a common vertex with C_g. After applying M_1-transformation, the trees are reduced to some stars with centers on C_g and the SK_1 index strictly increases by Lemma 7. Since $SK_1(A)$ is the maximum, it implies that $A = X(r, g; r_1, \ldots, r_g)$ where $r_1, \ldots, r_g \geq 0$ and $r_1 + \ldots + r_g = r - g$. All the pendant edges attached at the vertices of C_g are made incident to the unique and same vertex. After applying M_2, M_3-transformations several times, that would give $A = X_{r,g} = X(r, g; r-g, 0, \ldots, 0)$. □

Remark 2. *If $r-1 \geq g \geq 3$ then $SK_1(X(r, g; r-g, 0, \ldots, 0)) > SK_1(X(r, g+1; r-g-1, 0, \ldots, 0))$ by Case 1 of Lemma 7.*

Lemma 12. *(1) For $p = r - g \geq 3$, we have*

$$SK_1(A_2) < SK_1(A_1)$$

(2) For $p = r - g \geq 2$, we have

(a) $SK_1(A_3) < SK_1(A_1)$.
(b) $SK_1(A_4) < SK_1(A_1)$.
(c) $SK_1(A_5) < SK_1(A_1)$.

See Figure 6.

Proof.

$$\begin{aligned}
&SK_1(A_2) - SK_1(A_1)\\
&= \tfrac{1}{2}\{(2)(\mu-2+2) + (\mu-2)(1)(\mu-2+2) + (\mu-2+2)(2) + (2)(4) + (4)(2) + (4)(2)\}\\
&-\tfrac{1}{2}\{(2)(\mu-1+2) + (\mu-1)(1)(\mu-1+2) + (\mu-1+2)(3) + (3)(1) + (3)(2) + (2)(2)\}\\
&= \tfrac{1}{2}(-3\mu+7) < 0.
\end{aligned}$$

$$\begin{aligned}
&(a)\ SK_1(A_3) - SK_1(A_1)\\
&= \tfrac{1}{2}\{(\mu-1)(1)(\mu-1+2) + (\mu-1+2)(2) + (2)(3) + (3)(1) + (3)(2)\}\\
&-\tfrac{1}{2}\{(\mu-1)(1)(\mu-1+2) + (\mu-1+2)(3) + (3)(1) + (3)(2) + (2)(2)\}\\
&= \tfrac{1}{2}(-\mu+1) < 0.
\end{aligned}$$

$$\begin{aligned}
&(b)\ SK_1(A_4) - SK_1(A_1)\\
&= \tfrac{1}{2}\{(2+\mu-1)(2) + (\mu-2)(1)(\mu-2+3) + (\mu-2+3)(2) + (2)(1) + (\mu-1+2)(2)\\
&+(2)(2)\} - \tfrac{1}{2}\{(2+\mu-1)(2) + (\mu-1)(1)(\mu-1+2) + (\mu-1+2)(3) + (3)(1) + (3)(2)\}\\
&= -\tfrac{3}{2} < 0.
\end{aligned}$$

$(c)\ SK_1(A_5) - SK_1(A_1)$
$= \frac{1}{2}\{(2)(3) + (3)(\mu - 1 + 1) + (\mu - 1)(1)(\mu - 1 + 1) + (3)(2) + (2)(2)\}$
$-\frac{1}{2}\{(2)(\mu - 1 + 2) + (\mu - 1)(1)(\mu - 1 + 2) + (\mu - 1 + 2)(3) + (3)(1) + (3)(2)\}$
$= \frac{1}{2}(-3\mu + 3) < 0.$ □

Theorem 6. *(a) Let $A \in O_{r,g} \backslash \{X_{r,g}\}$, where $r \geq 6, (4 \leq g \leq r-2)$. Then A has a maximum SK_1 index if, and only if, $A = A_1$.*

(b) Let $A \in O_{r,g} \backslash \{(A_1 \cup X_{r,g})\}$, where $r \geq 7, (4 \leq g \leq r-3)$. Then A has a maximum SK_1 index if, and only if, $A = X(r, g; r-g-1, 0, 1, 0, \ldots, 0) = A_3$.

Proof. Let $A \in O_{r,g}$ be a connected unicyclic graph having the second or third maximum SK_1 index. Suppose that there is a vertex with a degree of at least 3 in a cycle C_g of A. Since $A \neq X_{r,g}$, then there is at least one non-pendant vertex in C.

Case 1: When there is exactly one non-pendant vertex outside C, we obtained A by attaching the μ pendant edges to a pendant vertex of $X(r-\mu, g; r-g-\mu, 0, \ldots, 0)$ where $(1 \leq \mu \leq r-g-1)$.

Lemma 11 states that for $\mu = 1$ or $r-4$ we have the maximum of $SK_1(U_r(\mu))$ with corresponding graphs A_4 and A_5.

However, Lemma 12 implies that the graphs with the second or third maximum SK_1 index, cannot be A_4 or A_5.

Case 2: When there are at least two non-pendant vertices outside C, after the continuous application of M_1-transformation, we have

$$SK_1(A) < max\{SK_1(A_4), SK_1(A_5)\} < SK_1(A_3) < SK_1(A_1) < SK_1(X_{r,g})$$

$$\text{as } SK_1(A_1) - SK_1(X_{r,g}) = \{\tfrac{1}{2}(r^2 + g^2 + 5r - g - 2rg + 1)\} - \{\tfrac{1}{2}(r^2 + g^2 + 6r - 2g - 2rg)\} = \tfrac{1}{2}(-r + g + 1) < 0$$

Thus, we knew that if A has a second or third maximum SK_1 index then the two vertices on C_g must exist having a degree of at least three.

(a) For $A \neq X_{r,g}$, if A has a maximum SK_1 then C_g cannot have three vertices with a degree of at least 3.

We obtained $X_{r,g}$ after several applications of M_i-transformations $(i \geq 1)$. However, we found a graph with an index less than $X_{r,g}$, we see that

$$SK_1(A) < max\{SK_1(A_3), SK_1(A_1)\} = SK_1(A_1) < SK_1(X_{r,g})$$

It implies that A has exactly two vertices m, n on C_g having a degree of at least 3.

Degrees of m and n must be as: $d(m) = r - g + 1, d(n) = 3$, since other cases cannot hold because if $d(m) = 2$ then A becomes $X_{r,g}$ (since our supposition of degree is at least 3) and if $d(m) = 4$ then A cannot become the second maximum because A with $d(m) = 3$ has a greater index than A with $d(m) = 4$.

Now, if $d(m, n) = 1$ then $A = A_1$ and if $d(m, n) \geq 2$ then $A \in Y(r, g)$ class including A_3. Lemma 12 implies that, in this case, the extremal graph is A_1.

(b) For $A \in O_{r,g} \backslash (A_1 \cup X_{r,g})$, by the same argument we deduce that C_g cannot have three vertices with a degree of at least 3, if A has a maximum SK_1 index, since, in this case, we would have

$$SK_1(A) < SK_1(A_3) < SK_1(A_1) < SK_1(X_{r,g})$$

$$\text{as } SK_1(A_3) - SK_1(A_1) = \{\tfrac{1}{2}(r^2 + g^2 + 4r - 2rg + 2)\} - \{\tfrac{1}{2}(r^2 + g^2 + 5r - g - 2rg + 1)\} = \tfrac{1}{2}(-r + g + 2) < 0$$

It implies that A has exactly two vertices a, b on C_g having a degree of at least 3. By the same argument (used above), $d(m) = r - g$ and $d(n) = 4$.

If $d(m,n) = 1$ then $A = A_6$ and if $d(m,n) \geq 2$ then $A \in Z(r,g)$ class including A_2, which ends the proof. □

(See Figure 10.)

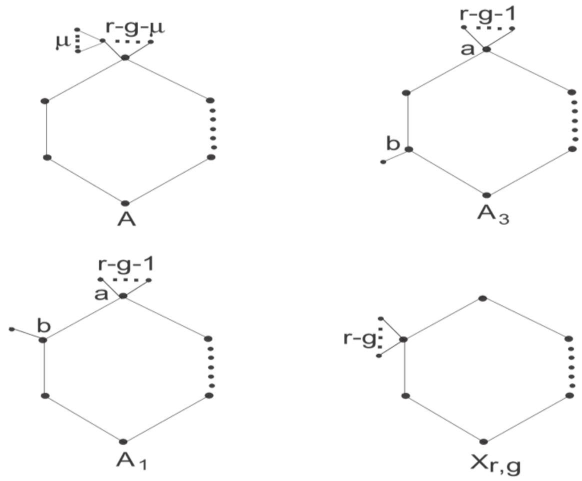

Figure 10. Unicyclic connected graphs having greatest SK_1 and SK_2 indices.

4. Ordering Unicyclic Structures with the Greatest SK_2 Index

In this section, we use graph transformations which increase the SK_2 index.

Lemma 13. *Let $M_1(A)$ be a unicyclic connected graph as shown in Figure 1, then*

$$SK_2(A) < SK_2(M_1(A))$$

for any $\mu, v \geq 0$.

Proof. Case 1: Ref. [19] When M_1 is performed excluding the vertices of C_g

$$\begin{aligned} SK_2(A) - SK_2(M_1(A)) &= \frac{1}{4}\sum_{xy\in E(A)\backslash\{yz\}}[(d_x+d_y)^2-(d_x+d_y+d_z-1)^2] \\ &+\frac{1}{4}\sum_{xz\in E(A)\backslash\{yz\}}[(d_x+d_z)^2-(d_x+d_y+d_z-1)^2] < 0;\ as\ d_y \geq 2 \end{aligned}$$

Case 2: When M_1 is performed on the vertices of C_g

We have $d_A(\omega_i) = d_{M_1(A)}(\omega_i) - v - 1 < d_{M_1(A)}(\omega_i)$ and $d_{M_1(A)}(\omega_i) + d_{M_1(A)}(\omega_{i+1}) = \mu + v + 4$.

Therefore, for $j = 1, \mu = 1, 2, \ldots, \mu$, $k = \overline{1, v} = 1, 2, \ldots, v$ and by the definition of the SK_2 index, we find

$$\begin{aligned} SK_2(A) - SK_2(M_1(A)) &= \tfrac{1}{4}[\{d(\omega_{i-1})+d(\omega_i)\}^2+\mu\{d(\omega_{i,j})+d(\omega_i)\}^2+\{d(\omega_i) \\ &+d(\omega_{i+1})\}^2+\nu\{d(\omega_{i+1,k})+d(\omega_{i+1})\}^2+\{d(\omega_{i+1})+d(\omega_{i+2})\}^2] \\ &-\tfrac{1}{4}[\{d(\omega_{i-1})+d(\omega_i)\}^2+(\mu+\nu+1)\{d(\omega_{i,j})+d(\omega_i)\}^2 \\ &+\{d(\omega_i)+d(\omega_{i+2})\}^2] \\ &= \tfrac{1}{4}\{(2+\mu+2)^2+\mu(1+\mu+2)^2+(\mu+2+\nu+2)^2+\nu(1+\nu+2)^2 \\ &+(\nu+2+2)^2\}-\tfrac{1}{4}\{(2+\mu+\nu+1+2)^2+(\mu+\nu+1) \\ &(1+\mu+\nu+1+2)^2+(\mu+\nu+1+2+2)^2\} \\ &= -\tfrac{1}{4}(3\mu^2+3\nu^2+19\mu+19\nu+20\mu\nu+3\mu^2\nu+3\mu\nu^2+18) < 0. \end{aligned}$$

$$\Rightarrow SK_2(A) < SK_2(M_1(A))\ \square$$

Lemma 14. *Let $M_2(A)$ be a unicyclic connected graph as depicted in Figure 2, where $d_A(\omega_i, \omega_{i+1}) = 1$. Then*

$$SK_2(A) < SK_2(M_2(A))$$

for any $v \geq \mu \geq 1$.

Proof. Since $d_{M_2(A)}(\omega_i) = 2 < d_A(\omega_i) = \mu + 2$ and $d_A(\omega_{i+1}) = \nu + 2 < d_{M_2(A)}(\omega_{i+1}) = \nu + \mu + 2$.

$$\begin{aligned} SK_2(A) - SK_2(M_2(A)) &= \tfrac{1}{4}[\{d(\omega_{i-1}) + d(\omega_i)\}^2 + \sum_{j=1}^{\mu} \{d(\omega_{i,j}) + d(\omega_i)\}^2 + \{d(\omega_i) \\ &+ d(\omega_{i+1})\}^2 + \sum_{k=1}^{\nu} \{d(\omega_{i+1,k}) + d(\omega_{i+1})\}^2 + \{d(\omega_{i+1}) + d(\omega_{i+2})\}^2] \\ &- \tfrac{1}{4}[\{d(\omega_{i-1}) + d(\omega_i)\}^2 + \{d(\omega_i) + d(\omega_{i+1})\}^2 \\ &+ (\mu+\nu)\{d(\omega_{i,j}) + d(\omega_{i+1})\}^2 + \{d(\omega_{i+1}) + d(\omega_{i+2})\}^2] \\ &= \tfrac{1}{4}[\{d(\omega_{i-1}) + d(\omega_i)\}^2 + \mu\{d(\omega_{i,j}) + d(\omega_i)\}^2 + \{d(\omega_i) \\ &+ d(\omega_{i+1})\}^2 + \nu\{d(\omega_{i+1,k}) + d(\omega_{i+1})\}^2 + \{d(\omega_{i+1}) + d(\omega_{i+2})\}^2] \\ &- \tfrac{1}{4}[\{d(\omega_{i-1}) + d(\omega_i)\}^2 + \{d(\omega_i) + d(\omega_{i+1})\}^2 \\ &+ (\mu+\nu)\{d(\omega_{i,j}) + d(\omega_{i+1})\}^2 + \{d(\omega_{i+1}) + d(\omega_{i+2})\}^2] \\ &= \tfrac{1}{4}\{(2+\mu+2)^2 + \mu(1+\mu+2)^2 + (\mu+2+\nu+2)^2 + \nu \\ &(1+\nu+2)^2 + (\nu+2+2)^2\} - \tfrac{1}{4}\{(2+2)^2 + (2+\mu+\nu+2)^2 \\ &+ (\mu+\nu)(1+\mu+\nu+2)^2 + (\mu+\nu+2+2)^2\} \\ &= -\tfrac{\mu\nu}{4}(3\mu + 3\nu + 14) < 0 \; for \; \nu \geq \mu \geq 1. \end{aligned}$$

$$\Rightarrow SK_2(A) < SK_2(M_2(A)) \; \square$$

Lemma 15. *Let $M_3(A)$ be a unicyclic connected graph as presented in Figure 3, where $d_A(\omega_i, \omega_{i+1}) = d_{M_3(A)}(\omega_i, \omega_{i+1}) \geq 2$. Then*

$$SK_2(A) < SK_2(M_3(A)); v \geq \mu \geq 1$$

Proof. Following the previous lemma and by the definition of $SK_2(A)$, we find

$$\begin{aligned} SK_2(A) - SK_2(M_3(A)) &= \tfrac{1}{4}[\{d(\omega_{i-1}) + d(\omega_i)\}^2 + \sum_{k=1}^{\mu} \{d(\omega_{i,j}) + d(\omega_i)\}^2 \\ &+ \{d(\omega_i) + d(\omega_{i+1})\}^2 + \{d(\omega_{i+1}) + d(\omega_j)\}^2 + \sum_{l=1}^{\nu} \{d(\omega_{j,\nu}) + d(\omega_j)\}^2 \\ &+ \{d(\omega_j) + d(\omega_{j+1})\}^2] - \tfrac{1}{4}[\{d(\omega_{i-1}) + d(\omega_i)\}^2 + \sum_{k=1}^{\mu-1} \\ &\{d(\omega_{i,\mu-1}) + d(\omega_i)\}^2 + \{d(\omega_i) + d(\omega_{i+1})\}^2 + \{d(\omega_{i+1}) \\ &+ d(\omega_j)\}^2 + \sum_{l=1}^{\nu+1} \{d(\omega_{j,\nu}) + d(\omega_j)\}^2 + \{d(\omega_j) + d(\omega_{j+1})\}^2] \\ &= \tfrac{1}{4}[\{d(\omega_{i-1}) + d(\omega_i)\}^2 + \mu\{d(\omega_{i,j}) + d(\omega_i)\}^2 \\ &+ \{d(\omega_i) + d(\omega_{i+1})\}^2 + \{d(\omega_{i+1}) + d(\omega_j)\}^2 + \nu\{d(\omega_{j,\nu}) + d(\omega_j)\}^2 \\ &+ \{d(\omega_j) + d(\omega_{j+1})\}^2] - \tfrac{1}{4}[\{d(\omega_{i-1}) + d(\omega_i)\}^2 + (\mu-1) \\ &\{d(\omega_{i,\mu-1}) + d(\omega_i)\}^2 + \{d(\omega_i) + d(\omega_{i+1})\}^2 + \{d(\omega_{i+1}) \\ &+ d(\omega_j)\}^2 + (\nu+1)\{d(\omega_{j,\nu}) + d(\omega_j)\}^2 + \{d(\omega_j) + d(\omega_{j+1})\}^2] \\ &= \tfrac{1}{4}\{(2+\mu+2)^2 + \mu(1+\mu+2)^2 + (\mu+2+2)^2 + (2+\nu+2)^2 \\ &+ \nu(1+\nu+2)^2 + (\nu+2+2)^2\} - \tfrac{1}{4}\{(2+\mu-1+2)^2 \\ &+ (\mu-1)(1+\mu-1+2)^2 + (\mu-1+2+2)^2 + (2+1+\nu+2)^2 \\ &+ (\nu+1)(1+\nu+1+2)^2 + (\nu+1+2+2)^2\} \\ &= \tfrac{1}{4}[(\mu-\nu)\{3\mu + 3\nu + 13\} - 6\nu - 7] < 0 \; \nu \geq \mu \geq 1. \end{aligned}$$

$$\Rightarrow SK_2(A) < SK_2(M_3(A)) \square$$

Hence, the proof is complete.

Lemma 16. *Let $M_4(A)$ be the graph as illustrated in Figure 4. For any $\nu \geq \mu \geq 1$, we have*

$$SK_2(A) < SK_2(M_4(A))$$

Proof. If $d_A(\omega_i, \omega_{i+1}) = 1$ then $d_{M_4(A)}(\omega_i) + d_{M_4(A)}(\omega_{i+1}) = \mu + 2 + v + 2 = d_A(\omega_i) + d_A(\omega_j)$ and by the definition of $SK_2(A)$, we have

$$\begin{aligned}
SK_2(A) - SK_2(M_4(A)) \quad &= \tfrac{1}{4}[\{d(\omega_{i-1}) + d(\omega_i)\}^2 + \sum_{j=1}^{\mu} \{d(\omega_{i,j}) + d(\omega_i)\}^2 + \{d(\omega_i) \\
&+d(\omega_{i+1})\}^2 + \sum_{k=1}^{\nu} \{d(\omega_{i+1,k}) + d(\omega_{i+1})\}^2 + \{d(\omega_{i+1}) + d(\omega_{i+2})\}^2] \\
&-\tfrac{1}{4}[\{d(\omega_{i-1}) + d(\omega_i)\}^2 + \sum_{j=1}^{\mu-1} \{d(\omega_{i,\mu-1}) + d(\omega_i)\}^2 + \{d(\omega_i) \\
&+d(\omega_{i+1})\}^2 + \sum_{k=1}^{\nu+1} \{d(\omega_{i+1,k}) + d(\omega_{i+1})\}^2 + \{d(\omega_{i+1}) + d(\omega_{i+2})\}^2] \\
&= \tfrac{1}{4}[\{d(\omega_{i-1}) + d(\omega_i)\}^2 + \mu\{d(\omega_{i,j}) + d(\omega_i)\}^2 + \{d(\omega_i) \\
&+d(\omega_{i+1})\}^2 + \nu\{d(\omega_{i+1,k}) + d(\omega_{i+1})\}^2 + \{d(\omega_{i+1}) + d(\omega_{i+2})\}^2] \\
&-\tfrac{1}{4}[\{d(\omega_{i-1}) + d(\omega_i)\}^2 + (\mu-1)\{d(\omega_{i,\mu-1}) + d(\omega_i)\}^2 + \{d(\omega_i) \\
&+d(\omega_{i+1})\}^2 + (\nu+1)\{d(\omega_{i+1,k}) + d(\omega_{i+1})\}^2 + \{d(\omega_{i+1}) + d(\omega_{i+2})\}^2] \\
&= \tfrac{1}{4}\{(2+\mu+2)^2 + \mu(1+\mu+2)^2 + (\mu+2+\nu+2)^2 + \nu \\
&(1+\nu+2)^2 + (\nu+2+2)^2\} - \tfrac{1}{4}\{(2+\mu-1+2)^2 + (\mu-1) \\
&(1+\mu-1+2)^2 + (\mu-1+2+\nu+1+2)^2 + (\nu+1) \\
&(1+\nu+1+2)^2 + (\nu+1+2+2)^2\} \\
&= \tfrac{1}{4}[(\mu-\nu)\{3(\mu+\nu)+11\} - 6\nu - 14] < 0 \; for \; \nu \geq \mu \geq 1.
\end{aligned}$$

$$\Rightarrow SK_2(A) < SK_2(M_4(A)) \square$$

Now first, we find the extremal graphs having the greatest value and then give an ordering of the unicyclic connected graphs in decreasing order for the SK_2 index.

Theorem 7 (Ref. [19]). *Let$X(r,3;a,b,c)$; $a+b+c = r-3$; $a \geq b \geq c \geq 1$ be a set of unicyclic connected graphs withr ≥ 5. Then the first maximum and second maximum values of theSK_2 index are attained by$X(r,3;r-3,0,0)$ and$X(r,3;r-4,1,0)$, respectively,i.e.,*

$$SK_2(X(r,3;r-4,1,0)) < SK_2(X(r,3;r-3,0,0))$$

See Figure 10.

Proof. We need only to prove $SK_2(X(r,3;a,b,c)) < SK_2(X(r,3;a+1,b-1,c))$.

$$\begin{aligned}
&SK_2(X(r,3;a,b,c)) - SK(X_2(r,3;a+1,b-1,c)) \\
&= \tfrac{1}{4}\{a(1+a+2)^2 + (a+2+b+2)^2 + b(1+b+2)^2 + (b+2+c+2)^2 + c(1+c+2)^2 \\
&+(c+2+a+2)^2\} - \tfrac{1}{4}\{(a+1)(1+a+1+2)^2 + (a+1+2+b-1+2)^2 \\
&+(b-1)(1+b-1+2)^2 + (b-1+2+c+2)^2 + c(1+c+2)^2 + (c+2+a+1+2)^2\} \\
&= \tfrac{1}{4}(-3a^2 + 3b^2 - 17a + 11b - 14) < 0 \; for \; a \geq b \geq c \geq 1.
\end{aligned} \quad \square$$

Hence, the result follows.

Lemma 17 (Ref. [19]). *If $SK_2(U_r(\mu))$ is the maximum for fixed $r \geq 5$, where $1 \leq \mu \leq r-4$, then we have $\mu = 1$ or $r-4$.*

Proof. For $r = 5$, $\mu = 1 = r-4$ and there is only one graph $U_5(1)$. Therefore, there cannot be a debate in choosing the maximum or minimum.

Suppose that $3 \leq \mu \leq r-5$, then

$$\begin{aligned} SK_2(U_r(\mu)) &= \tfrac{1}{4}\{2(2+r-\mu-4+3)^2+(r-\mu-4)(1+r-\mu-4+3)^2 \\ &\quad +(r-\mu-4+3+\mu+1)^2+\mu(1+\mu+1)^2+(2+2)^2\} \\ &= \tfrac{1}{4}(r^3-r^2+2\mu^2-3r^2\mu+3r\mu^2+4r+4r\mu+18) \end{aligned}$$

$$SK_2(U_r(\mu+1)) = \tfrac{1}{4}(r^3+2r^2+8\mu^2-3r^2\mu+3r\mu^2+7r+12\mu-2r\mu+34)$$

By using the above calculations, we determine

$$SK_2(U_r(\mu+1)) - SK_2(U_r(\mu)) = \frac{1}{4}(3r^2+6\mu^2+3r+12\mu-6r\mu+16) > 0$$

$$\Rightarrow SK_2(U_r(\mu+1)) > SK_2(U_r(\mu))$$

concluding that $SK_2(U_r(\mu)) > SK_2(U_r(r-4))$
where

$$\begin{aligned} SK_2(U_r(r-4)) &= \tfrac{1}{4}\{2(2+3)^2+(3+r-4+1)^2+(r-4)(1+r-4+1)^2+(2+2)^2\} \\ &= \tfrac{1}{4}(r^3-7r^2+20r+50) \end{aligned}$$

For $\mu = 1,2$, we have

$$SK_2(U_r(1)) = \tfrac{1}{4}(r^3-4r^2+11r+20)$$

$$SK_2(U_r(2)) = \tfrac{1}{4}(r^3-7r^2+24r+26)$$

Furthermore

$$SK_2(U_r(1)) - SK_2(U_r(2)) = \frac{1}{4}(3r^2-13r-6) > 0$$

$$SK_2(U_r(1)) - SK_2(U_r(r-4)) = \frac{1}{4}(3r^2-9r-30) > 0$$

$$SK_2(U_r(2)) - SK_2(U_r(r-4)) = r-6 > 0$$

By the above inequalities, we have

$$SK_2(U_r(1)) > SK_2(U_r(2)) > SK_2(U_r(\mu)) > SK_2(U_r(r-4)), U_r(\mu); 3 \leq \mu \leq r-5 \ \square$$

The above used graphs are shown in Figure 8. Therefore, $U_r(1)$ is a graph with the first maximum and $U_r(2)$ with the second maximum SK_2 index, andwe are complete.
Theorem 8. *Let A having girth g with $4 \leq g \leq r$, be a connected unicyclic graph. Then*

$$SK_2(A) \leq SK_2(X_{r,g})$$

where $X_{r,g} = X(r,g;r-g,0,\ldots,0)$.

Proof. Let $A \in O_{r,g}$, where $O_{r,g}$ be the set of unlabelled connected unicyclic graphs having order r and girth g with $r \geq g > 3$. If $g = r$, then $A = C_g$; for $g = r-1$ then $A = X(r,r-1;1,0,\ldots,0)$. Suppose that $3 \leq g \leq r-2$ and A has the largest SK_2 index. A is a graph with some vertex disjoint trees having each a common vertex with C_g. After applying M_1-transformation, the trees are reduced to some stars with centers on C_g and the SK_2 index strictly increases by Lemma 13. Since $SK_2(A)$ is the maximum, it implies that $A = X(r,g;r_1,\ldots,r_g)$ where $r_1,\ldots,r_g \geq 0$ and $r_1+\ldots+r_g = r-g$. All the pendant edges attached at the vertices of C_g are made incident to the unique and same vertex. After applying the M_2, M_3-transformations several times, that would give $A = X_{r,g} = X(r, g; r-g, 0, \ldots, 0)$. □

Remark 3. *If $r-1 \geq g \geq 3$ then $SK_2(X(r, g; r-g, 0, \ldots, 0)) > SK_2(X(r, g+1; r-g-1, 0, \ldots, 0))$ by Case 1 of Lemma 13.*

Lemma 18. *For $p = r - g \geq 2$, we have*

(a) $SK_2(A_2) < SK_2(A_1)$.
(b) $SK_2(A_3) < SK_2(A_1)$.
(c) $SK_2(A_4) < SK_2(A_1)$.
(d) $SK_2(A_5) < SK_2(A_1)$.

See Figure 6.

Proof.

$$
\begin{aligned}
&(a)\ SK_2(A_2) - SK_2(A_1)\\
&= \tfrac{1}{4}\{(2+\mu-2+2)^2 + (\mu-2)(1+\mu-2+2)^2 + (\mu-2+2+2)^2 + (2+4)^2 + (4+2)^2\\
&+(4+2)^2\} - \tfrac{1}{4}\{(2+\mu-1+2)^2 + (\mu-1)(1+\mu-1+2)^2 + (\mu-1+2+3)^2 + (3+1)^2\\
&+(3+2)^2 + (2+2)^2\}\\
&= -\tfrac{3}{4}\{\mu(\mu+3) - 12\} < 0.
\end{aligned}
$$

$$
\begin{aligned}
&(b)\ SK_2(A_3) - SK_2(A_1)\\
&= \tfrac{1}{4}\{(\mu-1)(1+\mu-1+2)^2 + (\mu-1+2+2)^2 + (2+3)^2 + (3+1)^2 + (3+2)^2\}\\
&-\tfrac{1}{4}\{(\mu-1)(1+\mu-1+2)^2 + (\mu-1+2+3)^2 + (3+1)^2 + (3+2)^2 + (2+2)^2\}\\
&= \tfrac{1}{2}(-\mu+1) < 0.
\end{aligned}
$$

$$
\begin{aligned}
&(c)\ SK_2(A_4) - SK_2(A_1)\\
&= \tfrac{1}{4}\{(2+\mu-1+2)^2 + (\mu-2)(1+\mu-2+3)^2 + (\mu-2+3+2)^2 + (2+1)^2\\
&+(\mu-1+2+2)^2 + (2+2)^2\} - \tfrac{1}{4}\{(2+\mu-1+2)^2 + (\mu-1)(1+\mu-1+2)^2\\
&+(\mu-1+2+3)^2 + (3+1)^2 + (3+2)^2\}\\
&= -\tfrac{9}{2} < 0.
\end{aligned}
$$

$$
\begin{aligned}
&(d)\ SK_2(A_5) - SK_2(A_1)\\
&= \tfrac{1}{4}\{(2+3)^2 + (3+\mu-1+1)^2 + (\mu-1)(1+\mu-1+1)^2 + (3+2)^2 + (2+2)^2\}\\
&-\tfrac{1}{4}\{(2+\mu-1+2)^2 + (\mu-1)(1+\mu-1+2)^2 + (\mu-1+2+3)^2 + (3+1)^2 + (3+2)^2\}\\
&= -\tfrac{3}{4}\{(\mu-1)(\mu+4)\} < 0.
\end{aligned}
$$

□

Theorem 9. *(a) Let $A \in O_{r,g} \backslash \{X_{r,g}\}$,* where $r \geq 4, (4 \leq g \leq r)$. *Then A has a maximum SK_2 index if, and only if, $A = A_1$.*

(b) Let $A \in O_{r,g} \backslash \{(A_1 \cup X_{r,g})\}$, where $r \geq 4, (4 \leq g \leq r)$. Then A has a maximum SK_2 index if, and only if, $A = X(r, g; r-g-1, 0, 1, 0, \ldots, 0) = A_3$.

Proof. Let $A \in O_{r,g}$ be a connected unicyclic graph having a second or third maximum SK_2 index. Suppose that there is a vertex with a degree at of least 3 in a cycle C_g of A. Since $A \neq X_{r,g}$, then there is at least one non-pendant vertex in C.

Case 1: When there is exactly one non-pendant vertex outside C, we obtained A by attaching the μ pendant edges to a pendant vertex of $X(r-\mu, g; r-g-\mu, 0, \ldots, 0)$ where $(1 \leq \mu \leq r-g-1)$.

Lemma 17 states that for $\mu = 1$ or $r-4$ we have a maximum of $SK_2(U_r(\mu))$ with corresponding graphs A_4 and A_5, respectively.

However, Lemma 17 implies that the graphs with a second or third maximum SK_2 index, cannot be A_4 or A_5.

Case 2: When there are at least two non-pendant vertices outside C, after the continuous application of M_1-transformation, we have

$$SK_2(A) < max\{SK_2(A_4), SK_2(A_5)\} < SK_2(A_3) < SK_2(A_1) < SK_2(X_{r,g})$$

$$\text{as } SK_2(A_1) - SK_2(X_{r,g}) = \left\{\frac{1}{4}(r^3 - g^3 + 5r^2 + 5g^2 - 3r^2g + 3rg^2 + 14r + 2g - 10rg + 14)\right\}$$
$$-\left\{\frac{1}{4}(r^3 - g^3 + 8r^2 + 8g^2 - 3r^2g + 3rg^2 + 25r - 9g - 16rg)\right\}$$
$$= \frac{1}{4}(-3r^2 - 3g^2 - 11r + 11g + 6rg + 14) < 0$$

Thus, we knew that if A has a second or third maximum SK_2 index then the two vertices on C_g must exist having a degree of at least three.

(a) For $A \neq X_{r,g}$, if A has a maximum SK_2 then C_g cannot have three vertices with a degree of at least 3.

We obtained $X_{r,g}$ after several applications of M_i-transformations $(i \geq 1)$. However, we found a graph with an index less than $X_{r,g}$, we see that

$$SK_2(A) < max\{SK_2(A_3), SK_2(A_1)\} = SK_2(A_1) < SK_2(X_{r,g})$$

It implies that A has exactly two vertices m, n on C_g having a degree of at least 3.

Degrees of m and n must be as: $d(m) = r - g + 1, d(n) = 3$, since other cases cannot hold because if $d(m) = 2$ then A becomes $X_{r,g}$ (since our supposition of degree is at least 3) and if $d(m) = 4$ then A cannot become the second maximum because A with $d(m) = 3$ has a greater index than A with $d(m) = 4$.

Now, if $d(m, n) = 1$ then $A = A_1$ and if $d(m, n) \geq 2$ then $A \in Y(r, g)$ class including A_3.

Lemma 18 implies that extremal graph is A_1 in this case.

(b) For $A \in O_{r,g} \backslash (A_1 \cup X_{r,g})$, by the same argument we deduce that C_g cannot have three vertices with a degree of at least 3, if A has a maximum SK index, since, in this case, we would have

$$SK_2(A) < SK_2(A_3) < SK_2(A_1) < SK_2(X_{r,g})$$

as $SK_2(A_3) - SK_2(A_1) = \{\frac{1}{4}(r^3 - g^3 + 5r^2 + 5g^2 - 3r^2g + 3rg^2 + 12r + 4g - 10rg + 16)\} - \{\frac{1}{4}(r^3 - g^3 + 5r^2 + 5g^2 - 3r^2g + 3rg^2 + 14r + 2g - 10rg + 14)\} = \frac{1}{4}(-2r + 2g + 2) < 0$

It implies that A has exactly two vertices a, b on C_g having a degree of at least 3.

By the same argument (used above), $d(m) = r - g$ and $d(n) = 4$.

If $d(m, n) = 1$ then $A = A_6$ and if $d(m, n) \geq 2$ then $A \in Z(r, g)$ class including A_2, which ends the proof. □

(See Figure 10.)

Now we take some graph structures $\tau_1, \tau_2, \tau_3, \tau_4, \tau_5, \tau_6$ with order $r = 11$ and girth $g = 5$, shown in Figure 11. Numerical values of Shighalli–Kanabur invariants are shown in Table 1 for the above-mentioned graphic structures. We can see that these computations verify our main results in Theorems 3, 6 and 9. We have molecular structures of certain compounds in chemistry which represents some of the graphs of our research as shown in Figure 12.

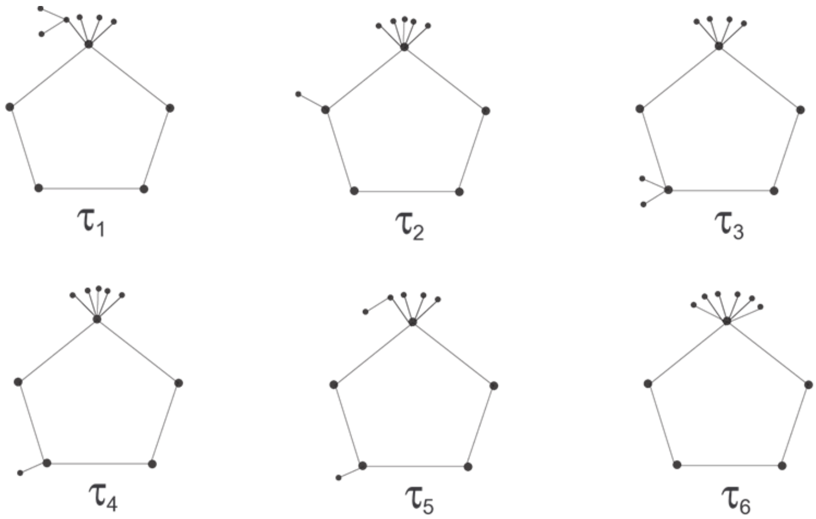

Figure 11. Unicyclic connected graphs having the greatest *SK* index.

Table 1. Comparison of different values of the SK, SK_1 and SK_2 indices.

Graphic Structure (τ)	SK (τ)	SK_1 (τ)	SK_2 (τ)
τ_1	33	39	109
τ_2	38	43.5	143.5
τ_3	35	38	115.5
τ_4	38	41	141
τ_5	33	44	107.5
τ_6	43	46	183.5

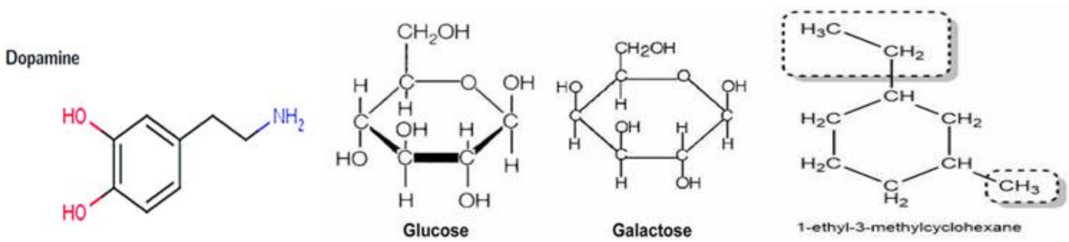

Figure 12. Molecular structures in chemistry.

These structures represents unicyclic graphs having pendant vertices, pendant edges, or pendant paths attached to the vertices of a cycle.

5. Conclusions

In this work, we determined the extremal unicyclic connected graphs of these certain degree-based chemical invariants, i.e., the SK index, the SK_1 index, and the SK_2 index of a given size, order, number of pendant vertices and girth by using some graph transformations. Furthermore, we presented an ordering giving a sequence of unicyclic connected graphs having these indices from greatest in decreasing order.

Author Contributions: Conceptualization, W.H., A.A., S.K., M.A., T.S.S. and X.Z.; methodology, A.A, S.K. and M.A.; validation, W.H., A.A., S.K., M.A., T.S.S. and X.Z.; formal analysis, A.A., S.K., T.S.S. and X.Z.; investigation, W.H., A.A. and S.K.; writing—original draft preparation, W.H., M.A., T.S.S. and X.Z.; writing—review and editing, A.A. and S.K. All authors have read and agreed to the published version of the manuscript.

Funding: This research project is supported by the Natural Science Foundation of Anhui Province Higher School (KJ2021A1154; 2022AH051864).

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. *Topological Indices, and Applications of Graph Theory*; Hindawi: London, UK, 2021.
2. Rouvray, D.H. The Search for Useful Topological Indices in Chemistry: Topological indices promise to have far-reaching applications in fields as diverse as bonding theory, cancer research, and drug design. *Am. Sci.* **1973**, *61*, 729–735.
3. Eliasi, M.; Taeri, B. Four new sums of graphs and their Wiener indices. *Discret. Appl. Math.* **2009**, *157*, 794–803. [CrossRef]
4. Gutman, I.; Trinajstic, N. Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* **1972**, *17*, 535–538. [CrossRef]
5. Khalifeh, M.H.; Yousefi-Azari, H.; Ashrafi, A.R. The first and second Zagreb indices of some graph operations. *Discret. Appl. Math.* **2009**, *157*, 804–811. [CrossRef]
6. Ghorbaninejad, M. The Zagreb-coindex of Four Operations on Graphs. *Fuzzy Optim. Model. J.* **2021**, *3*, 41–45.
7. Shigehalli, V.; Kanabur, R. New version of degree-based topological indices of certain nanotube. *J. Math. Nanosci.* **2016**, *6*, 27–40.
8. Kanabur, R.; Shigehalli, V. Computing Degree-Based Topological Indices of Polyhex Nanotubes. *J. Math. Nanosci.* **2016**, *6*, 47–55.
9. Shigehalli, V.S.; Kanabur, R. Computation of New Degree-Based Topological Indices of Graphene. *J. Math.* **2016**, *2016*, 4341919. [CrossRef]
10. Kang, S.M.; Zahid, M.A.; Virk, A.U.R.; Nazeer, W.; Gao, W. Calculating the Degree-based Topological Indices of Dendrimers. *Open Chem.* **2018**, *16*, 681–688. [CrossRef]
11. Ranjini, P.S.W.; Lokesha, V. *SK* Indices of Graph Operator *S(G)* and *R(G)* on few Nanostructures. *Montes Taurus J. Pure Appl. Math.* **2020**, *2*, 38–44.
12. Nurkahli, S.B.; Büyükköse, S. A Note on SK, SK_1 and SK_2 indices of Interval Weighted Graphs. *Adv. Inlinear Algebra Matrix Theory* **2021**, *11*, 14. [CrossRef]
13. Roy, K.; Ghosh, G. Exploring $QSAR_S$ with Extended Topochemical Atom (*ETA*) indices for modeling chemical and drug toxicity. *Curr. Pharm. Des.* **2010**, *16*, 2625–2639. [CrossRef] [PubMed]
14. Hosoya, H. Topological index as a sorting device for coding chemical structures. *J. Chem. Doc.* **1972**, *12*, 181–183. [CrossRef]
15. Hosoya, H. Graphical enumeration of the coefficients of the secular polynomials of the Hückel molecular orbitals. *Theor. Chim. Acta* **1972**, *25*, 215–222. [CrossRef]
16. Tomescu, I.; Kanwal, S. Unicyclic graphs of given girth $k = 4$ having smallest general sum-connectivity index. *Discret. Appl. Math.* **2014**, *164*, 344–348. [CrossRef]
17. Du, Z.; Zhou, B.; Trinajstić, N. Minimum general sum-connectivity index of unicyclic graphs. *J. Math. Chem.* **2010**, *48*, 697–703. [CrossRef]
18. Lokesha, V.; Yasmeen, K.Z. *SK* indices, forgotten topological indices and hyper Zagreb index of *Q* operator of carbon nanocone. *TWMS J. Appl. Eng. Math.* **2019**, *9*, 675–680.
19. Cancan, M.; Ediz, S.; Fareed, S.; Farahani, M.R. More topological indices of generalized prism network. *J. Inf. Optim. Sci.* **2020**, *41*, 925–932. [CrossRef]