Sanskruti Index of some Chemical Trees and Unicyclic Graphs

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Abstract. In chemical graph theory, topological indices are used to estimate the bio-activity of chemical compounds. The molecular graph models molecular compounds. A molecular graph represents the structural formula of a chemical compound relative to the graph. Its vertices represent the atoms of the compound, and its edges represent the chemical bonds. In 2017, Hosamani introduced the Sanskruti index $S(G)$ and defined it as $S(G) = \sum_{uv \in E(G)} \left( \frac{\delta_u \cdot \delta_v}{\delta_u + \delta_v - 2} \right)^3$, where $\delta_u$ is the sum of the degrees of all neighbors of the vertex $u$ in $G$. The Sanskruti index displays a good connection with an entropy of octane isomers. In this paper, the Sanskruti index $S(G)$ is computed for some chemical trees and unicyclic graphs.

1. Introduction

Let $G$ be a simple connected graph. $|V(G)|$ is the order of $G$, its number of vertices denoted by $n$. $|E(G)|$ is the size of a graph $G$, its number of edges denoted by $m$. The degree of a vertex $v$, indicated by $d(v)$. For a vertex $u$, we define $\delta_u = \sum_{v \in N_u} d(v)$, where $N_u$ denote the neighborhood of vertex $u$, this means $N_u = \{ v \in V(G) \mid uv \in E(G) \}$. A vertex has degree 0 said to be isolated, and a vertex has degree 1 to be a pendant vertex. A tree $T_n$ is a connected graph without any cycle. A tree of order $n$ with exactly two pendant vertices is said to be a path and denoted by $P_n$. The tree with $n - 1$ pendent vertices is a star of order $n$, denoted by $S_n$. A simple connected graph is called unicyclic if it has precisely one cycle [1].

Mathematical chemistry is a part of theoretical chemistry for studying and predicting the molecular structure utilizing mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a part of mathematical chemistry that uses graph theory in the mathematical modeling of chemical phenomena to develop the chemical sciences [2]. In mathematical chemistry, numbers encoding specific organic molecules' structural characteristics obtained from the corresponding molecular graph are named graph invariants or topological indices [3].

In 1947, topological indices were utilized in biology and chemistry for the first time when chemist Harold Wiener [4] presented the Wiener index to demonstrate correlations between properties of Physico-chemical for organic compounds of molecular graphs. Topological indices are numerical parameters of a graph that are invariant under the graphs' isomorphism [5]. Many topological indices can be introduced for the connected graph by different and various definitions. The connectivity index is one of the widely used to reflect molecular branching, introduced in 1975 by Randic [6], is defined as follows:
\[ R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u) \cdot d(v)}} \]

For the time being, there are several of these indices that have constructed applications in Mathematical chemistry. Most of these indices depend only on the degree of the vertex of the molecular graph. For example, the atom-bond connectivity index (\( ABC \)), presented by Estrada et al. [2]. It is defined as:

\[ ABC(G) = \sum_{uv \in E(G)} \left( \frac{d(u) \cdot d(v) - 2}{d(u) + d(v)} \right) \]

\( ABC \)-index gives a good model for the stability of branched and linear alkanes in addition to the stress-energy of cycloalkanes [2, 7]. Furtula et al. [8] introduced the improvement version of the \( ABC \)-index and named it the augmented Zagreb index (\( AZI \)):

\[ AZI(G) = \sum_{uv \in E(G)} \left( \frac{d(u) \cdot d(v)}{d(u) + d(v) - 2} \right)^3 \]

The predictive power is much better than the \( ABC \)-index in studying of formation heat of octane and heptane [8]. Motivated by previous researches on topological indices and their applications, Hosamani [9] defined the Sanskruti index \( S(G) \) for the molecular graph \( G \) as follows:

\[ S(G) = \sum_{uv \in E(G)} \left( \frac{\delta_u \cdot \delta_v}{\delta_u + \delta_v - 2} \right)^3 \quad (1) \]

\( S \)-index productivity was examined utilizing the isomers dataset, consisting of the following data: melting point, boiling point, molar refraction, heat capacities, acentric factor, octanol-water partition coefficient, total surface area, and entropy. The \( S \)-index correlated with all these properties, and the \( S \)-index has a good relationship with the octane isomers entropy, see Figure 1. The following structure-property relationship model was developed for the \( S \)-index [9].

\[ entropy = 1.7857 S \pm 81.4286I \]

![Figure 1](image_url)  
Figure 1. Correlation of \( S \)-index with the octane isomers entropy [9].

Sardar et al. computed the Sanskruti index of Polycyclic Aromatic Hydrocarbons [3]. Gao et al. presented explicit formulas for the Sanskruti index of an infinite group of dendrimer nanostars [10]. And, they computed the Sanskruti index for the Circumcoronene series of Benzenoid [11]. In this
paper, new theorems are presented with their proofs for the Sanskruti index for many important molecular graphs: caterpillar trees, cycle-caterpillar graphs, starlike trees and sunlike graphs.

2. Results
In this section, important classes of molecular graphs and their Sanskruti index are discussed.

**Proposition 1.** The Sanskruti index of the star graph $S_n$ is given by:

$$S(S_n) = \frac{(n-1)^7}{(2n-4)^3} \quad \text{Where } n \geq 3.$$  

**Proof.** In the graph $S_n$, there are $n - 1$ vertices with degree 1 which are $v_1, v_2, \ldots, v_{n-1}$ and one vertex $v_n$ with degree $n - 1$. Moreover, every vertex from the vertices $v_1, v_2, \ldots, v_{n-1}$, has one neighbor, which is a vertex $v_n$, this means $\delta(v_i) = n - 1, 1 \leq i \leq n - 1$. And, the vertex $v_n$ has $n - 1$ neighbors with degrees 1, this means $\delta(v_n) = n - 1$. Since the graph $S_n$ has $n - 1$ edges. So, we apply Equation (1):

$$S(S_n) = \sum_{v_i, v_j \in E(S_n)} \left( \frac{\delta(v_i) \cdot \delta(v_j)}{\delta(v_i) + \delta(v_j) - 2} \right)^3$$

$$= (n - 1) \left( \frac{(n-1)(n-1)}{n-1+n-1-2} \right)^3$$

$$= \frac{(n-1)^7}{(2n-4)^3}.$$

**Proposition 2.** The Sanskruti index of the path graph $P_n$ is satisfied with the following consequences:

1. $S(P_3) = 16$; 2. $S(P_4) = 27.39$; 3. $S(P_5) = 43.648$; and 4. $S(P_n) = 18.962n - 64.99$, where $n \geq 6$.

**Proof.** We can prove the points above (1, 2, and 3) directly using Equation (1). While point (4) can be proven as follows:

In the graph $P_n$, $n \geq 6$, there are $n - 4$ vertices with ($\delta = 4$) which are $v_3, v_4, \ldots, v_{n-3}, v_{n-2}$. And, two vertices ($v_2, v_{n-1}$) with ($\delta = 3$), also two vertices $v_1$ and $v_n$ with ($\delta = 2$). Moreover, there are $n - 1$ edges in $P_n$ which are $v_1v_2, v_2v_3, v_1v_{n-1}, \ldots, v_{n-2}v_{n-1}, v_{n-1}v_n$. So, we can apply Equation (1):

$$S(P_n) = \sum_{v_i, v_j \in E(P_n)} \left( \frac{\delta(v_i) \cdot \delta(v_j)}{\delta(v_i) + \delta(v_j) - 2} \right)^3$$

$$= \left( \frac{2 \cdot 3}{2+3-2} \right)^3 + \left( \frac{3 \cdot 4}{3+4-2} \right)^3 + \left( \frac{4 \cdot 4}{4+4-2} \right)^3 \cdots \left( \frac{4 \cdot 3}{4+3-2} \right)^3 \left( \begin{array}{c} n-5 \end{array} \right) \text{ times}$$

$$+ \left( \frac{3 \cdot 2}{3+2-2} \right)^3 = 18.962n - 64.99.$$

**Proposition 3.** The Sanskruti index of the cycle graph $C_n$ is given by:

$$S(C_n) = 18.962n, n \geq 3.$$  

**Proof.** In the graph $C_n$, every vertex $v_i, 1 \leq i \leq n$ has two neighbors with degrees 2. So, every vertex $v_i$ has ($\delta(v_i) = 4$). Moreover, the number of edges is equal to $n$. So, we can apply Equation (1):

$$S(C_n) = \sum_{v_i, v_j \in E(C_n)} \left( \frac{\delta(v_i) \cdot \delta(v_j)}{\delta(v_i) + \delta(v_j) - 2} \right)^3, \text{ where, } v_{n+1} = v_1$$

$$= n \left( \frac{4 \cdot 4}{4+4-2} \right)^3 = 18.962.$$

2.1. Caterpillar Trees and Cycle-caterpillars
Let $G$ be a labelled graph on $n$ vertices, and let $p_1, p_2, \ldots, p_n$ be non-negative integers. The thorn graph $G(p_1, p_2, \ldots, p_n)$ of the graph $G$ is obtained from $G$ by attaching $p_i$ pendant vertices to the $i$-th vertex of $G, i = 1, 2, \ldots, n$. The concept of thorn graphs was introduced by Gutman [12]. So, we can
define the caterpillar trees are thorn graphs whose parent graph is a path \( P_n \) and denoted by \( P^*_n = P_n (p_1, p_2, \cdots, p_n) \), see Figure 2. In other words, a caterpillar tree is a tree in which all the vertices are within distance 1 of the main path. If we delete all pendant vertices of a caterpillar tree, we reach a path [13].

**Remark 4.** It is easy to compute the Sanskruti index of caterpillar tree \( P^*_n, 1 \leq n \leq 4 \), directly. So, the Sanskruti index of \( P^*_n, n \geq 5 \) is computed in the theorem below.

![Figure 2. The caterpillar tree \( T_n(p_1, p_2, \cdots, p_{i+1}, \cdots, p_{n-1}, p_n) \)](image)

**Theorem 5.** Let \( P^*_n = P_n (p_1, p_2, \cdots, p_n) \) be the caterpillar tree, where \( p_1, p_2, \cdots, p_n \) are non-negative integers. The Sanskruti index of \( P^*_n \) is given by:

\[
S(P^*_n) = \sum_{k=1}^{10} A_k, \quad n \geq 5
\]

**Proof.** Let \( u_1, u_2, \cdots, u_n \) be the vertices of \( P_n \), and let \( v_1, v_2, \cdots, v_{p_i} \) be the pendant vertices to the \( i \)-th vertex of \( P^*_n \), where \( 1 \leq i \leq n \). The degree of the vertex \( u_i \), \( 2 \leq i \leq n - 1 \), is equal to \((2 + p_i)\), and the degrees of the vertices \( u_1 \) and \( u_n \) are equal to \( 1 + p_1 \) and \( 1 + p_n \), respectively. Moreover, there are two types of edges in the caterpillar tree \( P^*_n \): the first type is the edges between the vertices of \( P_n \), this means every edge \( u_iu_{i+1} \) has two ends in \( P_n \). And the second type is the edges that have one end \( u_i \) belongs to the vertices of \( P_n \) and the other end will be pendant vertex \( v_j, 1 \leq j \leq p_i \) (see Figure 2).

\[
A_1 = \left(\frac{(2+p_1+p_2)(3+p_1+p_2+p_3)}{3+p_1+2p_2+p_3}\right)^3, \quad A_2 = \left(\frac{(3+p_1+p_2)(4+p_1+p_2+p_3)}{5+p_1+2p_2+p_3}\right)^3,
\]
\[
A_3 = \left(\frac{(4+p_{n-1}+p_{n-2}+p_{n-3})(4+p_{n-2}+p_{n-1}+p_n)}{5+p_{n-3}+2p_{n-2}+2p_{n-1}+p_n}\right)^3,
\]
\[
A_4 = \left(\frac{(4+p_{n-2}+p_{n-1}+p_n)(2+p_{n-1}+p_n)}{3+p_{n-2}+2p_{n-1}+2p_n}\right)^3,
\]
\[
A_5 = \sum_{i=3}^{n-2} \left(\frac{(4+p_{i-1}+p_i)(4+p_{i+1})(4+p_{i+1}+p_{i+2})}{6+p_{i-1}+2p_i+2p_{i+1}+p_{i+2}}\right)^3,
\]
\[
A_6 = p_i \left(\frac{(2+p_1+p_2)(1+p_i)}{1+2p_1+p_2}\right)^3, \quad A_7 = p_2 \left(\frac{(3+p_1+p_2)(2+p_2)}{3+p_1+2p_2}\right)^3,
\]
\[
A_8 = p_{n-1} \left(\frac{(3+p_{n-2}+p_{n-1}+p_2)(2+p_{n-1})}{3+p_{n-2}+2p_{n-1}+p_n}\right)^3, \quad A_9 = p_n \left(\frac{(2+p_{n-1}+p_n)(1+p_n)}{1+p_{n-1}+2p_n}\right)^3,
\]
\[
A_{10} = \sum_{i=3}^{n-2} p_i \left(\frac{(4+p_{i-1}+p_i)(4+p_{i+1})(4+p_{i+1})}{4+p_{i-1}+2p_i+p_{i+1}}\right)^3.
\]

**Proof.** Let \( u_1, u_2, \cdots, u_n \) be the vertices of \( P_n \), and let \( v_1, v_2, \cdots, v_{p_i} \) be the attached pendant vertices to the \( i \)-th vertex of \( P^*_n \), where \( 1 \leq i \leq n \). The degree of the vertex \( u_i \), \( 2 \leq i \leq n - 1 \), is equal to \((2 + p_i)\), and the degrees of the vertices \( u_1 \) and \( u_n \) are equal to \((1 + p_1)\) and \((1 + p_n)\) respectively. Moreover, there are two types of edges in the caterpillar tree \( P^*_n \): the first type is the edges between the vertices of \( P_n \), this means every edge \( u_iu_{i+1} \) has two ends in \( P_n \). And the second type is the edges that have one end \( u_i \) belongs to the vertices of \( P_n \) and the other end will be pendant vertex \( v_j, 1 \leq j \leq \)
$p_i$ (see Figure 2). To compute the Sanskruti index of $P_n^*$, we must find the sum of the degrees of all neighbors of every vertex in $P_n^*$, this means finding $\delta$ for all vertices. The vertex $u_4$ has $p_1$ neighbors with degrees 1 and one neighbor $u_2$ with a degree $(2 + p_2)$. So, $\delta_{u_4} = 2 + p_1 + p_2$. The vertex $u_2$ has $p_2$ neighbors with degrees 1, one neighbor $u_4$ with a degree $(1 + p_2)$ and one neighbor $u_3$ with a degree $(2 + p_3)$. So, $\delta_{u_2} = 3 + p_1 + p_2 + p_3$. The vertex $u_4, 3 \leq i \leq n - 2$, has $p_i$ neighbors with degrees 1, one neighbor $u_{i-1}$ with degree $(2 + p_{i-1})$ and one neighbor $u_{i+1}$ with degree $(2 + p_{i+1})$. So, $\delta_{u_i} = 4 + p_{i-1} + p_i + p_{i+1}$. The vertex $u_{n-1}$ has $p_{n-1}$ neighbors with degrees 1, one neighbor $u_n$ with degree $(1 + p_n)$ and one neighbor $u_{n-2}$ with degree $(2 + p_{n-2})$. So, $\delta_{u_{n-1}} = 3 + p_{n-2} + p_{n-1} + p_1$. The vertex $u_n$ has $p_n$ neighbors with degrees 1 and one neighbor $u_{n-1}$ with degree $(1 + p_{n-1})$. So, $\delta_{u_n} = 2 + p_{n-1} + p_n$. Moreover, the pendant vertex $v_j, 1 \leq j \leq p_i, 2 \leq i \leq n - 1$ has one neighbor $u_i$ with a degree $(2 + p_i)$. So, $\delta_{v_j} = 2 + p_i$. But, the pendant vertex $v_r, 1 \leq r \leq p_1$, has one neighbor $u_1$ with a degree $(1 + p_1)$. So, $\delta_{v_r} = 1 + p_1$, and the pendant vertex $v_s, 1 \leq s \leq p_n$, has one neighbor $u_n$ with a degree $(1 + p_n)$. So, $\delta_{v_s} = 1 + p_n$. Now, we can apply Equation 1 to the first type of edges $u_i u_{i+1}$, to obtain the terms $A_k, 1 \leq k \leq 5$, and to the second type of edges $u_i v_j, 1 \leq j \leq p_i$, to obtain the term $A_k, 6 \leq k \leq 10$. Caterpillar trees are used in chemical graph theory to represent the structure of hydrocarbon molecules. For example, for positive integer $p_1 = p_2 = 3$ and $p_2 = p_3 = \cdots = p_{n-1} = 2$, the caterpillar tree $P_n(3, 2, 2, \cdots, 2, 3)$ is the molecular graph of certain hydrocarbon (straight-chain alkanes, a single chain with no branches, have the general chemical formula $C_nH_{2n+2}$), see Figure 3. It is easy to find the Sanskruti index of the molecular graphs of Ethane $P_2(3, 3)$, Propane $P_3(3, 2, 3)$, and Butane $P_4(3, 2, 2, 3)$ using Equation 1. So, Theorem 5 is used to get the formulae for the Sanskruti index of the straight-chain alkanes $C_nH_{2n+2} = P_n(3, 2, 2, \cdots, 2, 3), n \geq 5$, as shown in Corollary 6.

![Figure 3](image-url)  

**Figure 3.** The molecular graphs of hydrocarbon (straight-chain alkanes).

**Corollary 6.** The Sanskruti index of the straight-chain alkanes $C_nH_{2n+2} = P_n(3, 2, 2, \cdots, 2, 3), n \geq 5$, is given by:

$$S(C_nH_{2n+2}) = 199.074n - 120.354, n \geq 5$$

**Proof.** We used Theorem 5 and replaced $p_i$ with 2, 2 $\leq i \leq n - 1$, also replaced both $p_1$ and $p_n$ with 3.

A unicyclic graph is called a **cycle-caterpillar** if deleting all its pendent (end) vertices will reduce it to a cycle, and denoted by $C_n(p_1, p_2, \cdots, p_n)$. So, the cycle-caterpillars are thorn graphs whose parent graph is a cycle; see Figure 4.
Theorem 7. Let $C_n^* = C_n(p_1, p_2, \ldots, p_n)$ be the cycle-caterpillar, and $p_1, p_2, \ldots, p_n$ are non-negative integers. The Sanskruti index of $C_n^*$ is given by:

$$S(C_n^*) = B_1 + B_2$$

Where,

$$B_1 = \sum_{i=1}^{n} \left( \frac{(4+p_{i-1}+p_{i}+p_{i+1})(4+p_{i}+p_{i+1}+p_{i+2})}{6+p_{i-1}+2p_{i}+2p_{i+1}+p_{i+2}} \right)^3, \text{ where } p_{n+1} = p_1$$

$$B_2 = \sum_{i=1}^{n} p_i \left( \frac{(4+p_{i-1}+p_{i}+p_{i+1})(2+p_i)}{4+p_{i-1}+2p_i+p_{i+1}} \right)^3, \text{ where } p_{n+1} = p_1$$

Proof. Let $u_1, u_2, \ldots, u_n$; un be the vertices of $C_n$, and let $v_1, v_2, \ldots, v_{p_i}$ be the attached pendant vertices to the $i$-th vertex of $C_n$, where $1 \leq i \leq n$. The degree of the vertex $u_i$, $1 \leq i \leq n$, is equal to $(2 + p_i)$. Moreover, there are two types of edges in cycle-caterpillar $C_n^*$: the first type is the edges between the vertices of $C_n$, this means every edge $u_i u_{i+1}$ has two ends in $C_n$. And the second type is the edges that have one end $u_i$ belongs to the vertices of $C_n$ and the other end will be pendant vertex $v_j$, $1 \leq j \leq p_i$ (see Figure 4). To compute the Sanskruti index of $C_n$, we must find the sum of the degrees of all neighbors of every vertex in $C_n$, this means finding $\delta$ for all vertices. The vertex $u_i$, $1 \leq i \leq n$, has $p_i$ neighbors with degrees 1, one neighbor $u_{i-1}$ with degree $(2 + p_{i-1})$ and one neighbor $u_{i+1}$ with degree $(2 + p_{i+1})$. So, $\delta_{u_i} = 4 + p_{i-1} + p_i + p_{i+1}$. Moreover, the pendant vertex $v_j$, $1 \leq j \leq p_i$, $1 \leq i \leq n$ has one neighbor $u_i$ with degree $(2 + p_i)$. So, $\delta_{v_j} = 2 + p_i$. Now, we can apply Equation 1 to the first type of edges $u_i u_{i+1}$, to obtain the term $B_1$, and to the second type of edges $u_i v_j$, to obtain the term $B_2$.

2.2. Starlike Trees and Sunlike Graphs

Let $v$ be an isolated vertex and let $P_1, P_2, \ldots, P_m$ be the paths of orders $n_1, n_2, \ldots, n_m$, where are the positive integers $n_i$, $1 \leq i \leq m$. The starlike tree $T_m(n_1, n_2, \ldots, n_m)$ is the tree obtained by identifying the end vertex $v_i$ of $P_i$, with the vertex $u$ for all $i = 1, 2, \ldots, m$. 

Figure 4. The cycle-caterpillar $C_n(p_1, p_2, \ldots, p_n)$.
In other words, a starlike tree is a tree with exactly one vertex $u$ having a degree of at least 3 and has the property that $T_m(n_1, n_2, \ldots, n_m) - u = P_1 \cup P_2 \cup \cdots \cup P_m$, where $|P_i| = n_i$, $n_i \geq 1$, $1 \leq i \leq m$, see Figure 5. The vertex $u$ will be the center of the starlike tree. And $v_j$ means the vertex $v$ at the $j$-th position of the $i$ path $(P_i)$, $1 \leq i \leq m$, $1 \leq j \leq n_i$. Clearly, for $n_i \geq 1$, $d(v_{im}) = 1$. Theorem 8. Let $T_m^* = T_m(n_1, n_2, \ldots, n_m)$ be the starlike tree, and $l$ be the biggest order such that $l \geq n_i$, $1 \leq i \leq m$.

\textbf{Proof.} Let the vertex $u$ be the center of $T_m^*$ (it is clear that, $T_m^*$ has $m$ paths). To compute the Sanskruti index of $T_m^*$, we must find the sum of the degrees of all neighbors of every vertex in $P_m^*$, this means finding $\delta$ for all vertices. Since all neighbors of the center $u$ have degrees 2 except for the vertices $v_{1i}$ that belong. To $I_1$, $1 \leq i \leq m$ and $|I_1| = t_1$. Then, $\delta_{ui} = m - t_1$. Moreover, the vertex $v_{1i}$, $i \in I_1$, has only one neighbor, which is the vertex $u$, this means $\delta_{v_{1i}} = m = \delta_{v_{mi}}$. Also, the vertex $v_{il}$, $i \in I_2$, has two neighbors, which are the vertices $u$, and $v_{mi}$, this means $\delta_{v_{il}} = m + 1$. Since every vertex $v_{ij}$, $1 \leq i \leq m$, $i \in I_3 \cup I_4 \cup A$, $2 \leq j \leq n_i - 1$, has degree 2, where $A = \bigcup_{4 \leq r \leq l} I_r$. Then, the vertex $v_{il}$ has two neighbors, which are the vertices $u$ and $v_{il}$, this means $\delta_{v_{il}} = m + 2$. Furthermore, the vertex $v_{il}^2$, $i \in I_2$, has only one neighbor, which is the vertex $v_{il}^1$, this means $\delta_{v_{il}^2} = 2 = \delta_{v_{il}^1}$. In general, $\delta_{v_{im}} = 2$, where $v_{mi}$ is the end vertex in the path $P_i$ with order $n_i$. Also, the vertex $v_{i(n_i-1)}$, $i \in I_3$, $\delta_{v_{i(n_i-1)}} = 2$.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{starlike_tree.png}
\caption{The starlike tree $T_m(n_1, n_2, \ldots, n_m)$.}
\end{figure}

In general, the Sanskruti index of $T_m^*$ is given by:

$$S(T_m^*) = \sum_{k=1}^{9} E_k,$$

Where,

$$E_1 = t_1 \left(\frac{2m-t_1}{2m-t_1-2}\right)^3, E_2 = t_2 \left(\frac{(2m-t_1)(m+1)}{3m-t_1-1}\right)^3,$$

$$E_3 = (m-t_1-t_2) \left(\frac{(2m-t_1)(m+2)}{3m-t_1}\right)^3,$$

$$E_4 = 8t_2, E_5 = t_3 \left(\frac{3m+6}{m+3}\right)^3, E_6 = (m-t_1-t_2-t_3) \left(\frac{4m+8}{m+4}\right)^3,$$

$$E_7 = 8(m-t_1-t_2), E_8 = 13.824(m-t_1-t_2-t_3),$$

$$E_9 = \sum_{4 \leq r \leq l, s \in r} 18.962t_r s.$$
has two neighbors, which are the vertices \( v_{in_1} \) with degree 1 and the vertex \( v_{(n_1-2)} \) with degree 2, this means \( \delta_{v_{(n_1-1)}} = 3 \). Finally, every vertex \( v_{ij}, i \in I_4 \cup A, 2 \leq j \leq n_1 - 2 \), has two neighbors, which are the vertices \( v_{(j-1)} \) with a degree 2 and the vertex \( v_{(j+1)} \) with a degree 2, this means \( \delta_{v_{ij}} = 4 \).

Now, we can apply Equation 1 to the first edges \( v_{11} \), \( 1 \leq i \leq m \) to obtain the terms \( E_1, E_2 \) and \( E_3 \):

\[
\sum_{i \in E_1} \left( \frac{\delta_u \delta_{v_{11}}}{\delta_u + \delta_{v_{11}} - 2} \right)^3 = E_1, \quad \sum_{i \in E_2} \left( \frac{\delta_u \delta_{v_{11}}}{\delta_u + \delta_{v_{11}} - 2} \right)^3 = E_2, \quad \sum_{i \in E_3} \left( \frac{\delta_u \delta_{v_{11}}}{\delta_u + \delta_{v_{11}} - 2} \right)^3 = E_3.
\]

And, we apply Equation 1 to the second edges \( v_{11}v_{12}, 1 \leq i \leq m, i \notin I_1 \), to obtain the terms \( E_4, E_5 \), and \( E_6 \). If \( i \in I_2 \), then the second edges will be \( v_{11}v_{(n_1)} \), as shown in term \( E_4 \) below:

\[
\sum_{i \in E_4} \left( \frac{\delta_u \delta_{v_{11}}}{\delta_u + \delta_{v_{11}} - 2} \right)^3 = E_4, \quad \sum_{i \in E_5} \left( \frac{\delta_u \delta_{v_{11}}}{\delta_u + \delta_{v_{11}} - 2} \right)^3 = E_5, \quad \sum_{i \in E_6} \left( \frac{\delta_u \delta_{v_{11}}}{\delta_u + \delta_{v_{11}} - 2} \right)^3 = E_6.
\]

Also, we apply Equation 1 to the end edges \( v_{(n_1-1)}v_{n_1} \), \( 1 \leq i \leq m, i \in I_3 \cup I_4 \cup A \) (if \( i \in I_2 \), then the end edges will be the second edges \( v_{11}v_{12} \), as shown in term \( E_4 \) above), to obtain the term \( E_7 \):

\[
\sum_{i \in E_7} \left( \frac{\delta_u \delta_{v_{(n_1-1)}}}{\delta_u + \delta_{v_{(n_1-1)}} - 2} \right)^3 = E_7.
\]

Furthermore, we apply Equation 1 to the edges \( v_{(n_1-2)}v_{(n_1-1)} \), \( 1 \leq i \leq m, i \in I_3 \cup A \) (if \( i \in I_2 \), then the edges \( v_{(n_1-2)}v_{(n_1-1)} \) will be the second edges \( v_{11}v_{12} \), as shown in term \( E_5 \) above), to obtain the term \( E_8 \):

\[
\sum_{i \in E_8} \left( \frac{\delta_u \delta_{v_{(n_1-1)}}}{\delta_u + \delta_{v_{(n_1-1)}} - 2} \right)^3 = E_8.
\]

We calculated all edges of the path \( P_i, |P_i| = n_1 = 4 \), as shown in terms \( E_2, E_4, E_7 \) and \( E_8 \) above. Also, we calculated four edges from every path \( P_i, |P_i| = n_1 = 5 \), which are the first edges, second edges, last edges, and one previous. If \( |P_i| = n_1 = 5 \), then one edge still from \( P_i \). If \( |P_i| = n_1 = 6 \), then two edges still from \( P_i \). Generally, \( r - 4 \) still from the path \( P_i \), where \( |P_i| = n_1 = r \). Now, we apply Equation 1 to the edges \( v_{ij}v_{(i+1)(j+1)} \), \( 1 \leq i \leq m, 2 \leq j \leq n_1 - 3, n_1 > 4 \), this means \( i \in A \), to obtain the term \( E_9 \):

\[
\sum_{i \in E_9} \left( \frac{\delta_u \delta_{v_{(i+1)(j+1)}}}{\delta_u + \delta_{v_{(i+1)(j+1)}} - 2} \right)^3 = E_9.
\]

Where,

\[
\left( \frac{\delta_u \delta_{v_{(i+1)(j+1)}}}{\delta_u + \delta_{v_{(i+1)(j+1)}} - 2} \right)^3 = 18.962, \forall i, j.
\]

And, \( t_r \) is the number of paths \( P_i \) of order \( n_1 = r (|P_i| = t_r) \), \( 1 \leq i \leq m, 4 < r < l \).

Let \( C \) be a cycle on \( m \) vertices with the vertex set \( V(C) = \{u_1, u_2, \ldots, u_m\} \) and let \( P_1, P_2, \ldots, P_m \) be the paths of orders \( n_1, n_2, \ldots, n_m \), where \( n_i \) is the positive integers, \( 1 \leq i \leq m \). The sunlike graph \( U_m(n_1, n_2, \ldots, n_m) \) is the graph obtained by identifying the end vertex of \( P_i \) with the \( i \)-th vertex of \( C \) for all \( i = 1, 2, \ldots, m \), see Figure 6. In other words, a sunlike graph has the property that
\( U_m(n_1, n_2, \ldots, n_m) - C_m = P_1 \cup P_2 \cup \cdots \cup P_m \), where \( |P_i| = n_i, n_i \geq 1, 1 \leq i \leq m \). If the path \( P_i \) of order \( n_i \) is identifying with the vertex \( u_i \) of \( C_m \), then we denote the vertex \( u_i \) by \( u_i(n_i) \). Also, we define \( v_i(1) \) is the smallest vertex, this means the identification path \( P_i \) has order 1. Moreover, the vertex \( v_{ij} \) means the vertex \( v \) at the \( j \)-th position of the \( i \) path \( (P_i) \), \( 1 \leq j \leq n_i \). If \( n_i \geq 1, j = n_i \), then \( d(v_{in_i}) = 1 \).

**Figure 6.** The sunlike graph \( C_m(3,2, n_3, 3,1,4, \ldots, 2) \).

**Corollary 9.** Let \( U_m^{*} = U_m(n_1, n_2, \ldots, n_m) \) be the sunlike graph, and \( l \) be the biggest order such that \( l \geq n_i, 1 \leq i \leq m \). If \( I_1 = \{ i : 1 \leq i \leq m, n_i = 1, i.e., |P_i| = 1 \} \), \( I_2 = \{ i : 1 \leq i \leq m, n_i = 2 \} \), \( \ldots \), \( I_{l-1} = \{ i : 1 \leq i \leq m, n_i = l-1 \} \), \( I_l = \{ i : 1 \leq i \leq m, n_i = l \} \), where \( |I_1| = t_1, |I_2| = t_2, \ldots, |I_{l-1}| = t_{l-1}, |I_l| = t_l \). Then, the Sanskruti index of \( U_m^{*} \) is given by:

\[
S(U_m^{*}) = \sum_{k=1}^{12} H_k
\]

Where,

\[
H_1 = 18.087t_1, \quad H_2 = 17.576t_2, \quad H_3 = 48.084(m - t_1 - t_2).
\]

\[
H_4 = 15.625t_3, \quad H_5 = 15.625t_3, \quad H_6 = 23.323(m - t_1 - t_2 - t_3).
\]

\[
H_7 = 8(m - t_1 - t_2), \quad H_8 = 13.824(m - t_1 - t_2 - t_3), \quad H_9 = \sum_{s=2}^{m-r-4} 4.096t_r s .
\]

\[
H_{10} = 68.083f_1, \quad H_{11} = 79.934f_2, \quad H_{12} = 95.533(m - f_1 - f_2).
\]

While \( f_1 \) is the number of edges \( u_i u_{i+1} \) that have two smallest vertices \( u_i(1) \) and \( u_{i+1}(1) \). And, \( f_2 \) is the number of edges \( u_i u_{i+1} \) that have precisely one smallest vertex \( u_i(1) \) or \( u_{i+1}(1) \).

**Proof.** The proof method is the same as the proof method of Theorem 8, except for changing the vertex \( u \) in the starlike tree to the number of vertices \( u_1, u_2, \ldots, u_m \) in this graph (sunlike), and we calculate the new edges \( u_i u_{i+1} \) using Equation 1. Since \( m \) was the degree of vertex \( u \) in the starlike tree, but the degrees of \( u_1, u_2, \ldots, u_m \) are 3. Therefore, the calculation of the first and second edges (mentioned in the proof of Theorem 8) will change depending on the degree of vertex \( u \). So, if \( u_i = u_i(1) \) (the identification path \( P_i \) has order 1), then \( \delta_{u_i} = d(u_{i-1}) + d(u_{i+1}) + d(v_{i1}) = 7 \). And, \( \delta_{u_i} = 8 \) where \( u_i = u_i(n_i), n_i \geq 2, 1 \leq i \leq m \). Moreover, the vertex \( v_{11} \), \( i \in I_1 \), has only one neighbor, which is the vertex \( u_i(1) \) with degree 3, this means \( \delta_{v_{11}} = 3 = \delta_{v_{in_i}} \). Also, the vertex \( v_{11}, i \in I_2 \), has two neighbors, which are the vertices \( u_i, v_{in_i} \) with degree one, this means \( \delta_{v_{11}} = 4 \). Since every vertex \( v_{ij}, 1 \leq i \leq m, i \in I_2 \cup I_4 \cup A, 2 \leq j \leq n_i - 1 \), has degree 2, where \( A = \cup_{4 < r \leq l} I_r \). Then, the vertex \( v_{11} \) has two neighbors, which are the vertices \( u_i \) and \( v_{12} \), this means \( \delta_{v_{11}} = 4 \).
4. Furthermore, the vertex \( v_{i2} \), \( i \in I_2 \), has only one neighbor, which is the vertex \( v_{i1} \), this means \( \delta_{v_{i2}} = 2 = \delta_{v_{i1}} \). In general, \( \delta_{v_{in_i}} = 2 \), where \( v_{in_i} \) is the end vertex in the path \( P_i \) with order \( n_i \). Also, the vertex \( v_{i(n_i−1)} \), \( i \in I_3 \), has two neighbors, which are the vertices \( v_{in_i} \) with degree 1 and the vertex \( v_{i(n_i−2)} \) with degree 2, this means \( \delta_{v_{in_i−1}} = 3 \). Finally, every vertex \( v_{ij} \), \( i \in I_4 \cup A \), \( 2 ≤ j ≤ n_i − 2 \), has two neighbors, which are the vertices \( v_{i(j−1)} \) with a degree 2 and the vertex \( v_{i(j+1)} \) with a degree 2, this means \( \delta_{v_{ij}} = 4 \). Now, we can apply Equation 1 to the first edges \( u_i v_{i1}, 1 ≤ i ≤ m \), to obtain the terms \( H_1, H_2 \) and \( H_3 \):

\[
\sum_{i \leq i \leq m} \left( \frac{\delta_{u_i} \delta_{v_{i1}}}{\delta_{u_i} + \delta_{v_{i1}}} \right)^3 = H_1, \quad \sum_{i \leq i \leq m} \left( \frac{\delta_{u_i} \delta_{v_{i1}}}{\delta_{u_i} + \delta_{v_{i1}}} \right)^3 = H_2
\]

\[
\sum_{i \leq i \leq m} \left( \frac{\delta_{u_i} \delta_{v_{i1}}}{\delta_{u_i} + \delta_{v_{i1}}} \right)^3 = H_3
\]

The method used to obtain \( H_4, H_5, \ldots, H_9 \) is the same as the method used to obtain \( E_1, E_2, \ldots, E_9 \) in the proof of Theorem 8. Equation 1 is applied to the second edges \( v_{i2} \), \( 1 ≤ i ≤ m \), \( i \in I_1 \), to obtain the terms \( H_4 \) and \( H_5 \). Also, it is applied to the end edges \( v_{i(n_i−1)} \), \( 1 ≤ i ≤ m \), \( i \in I_3 \cup I_4 \cup A \), to obtain the term \( H_7 \). Moreover, Equation 1 is applied to the edges \( v_{i(n_i−2)} \), \( 1 ≤ i ≤ m \), \( i \in I_4 \cup A \), to obtain the term \( H_8 \). Also, it is applied to the edges \( v_{ij} v_{i(j+1)} \), \( 1 ≤ i ≤ m \), \( 2 ≤ j ≤ n_i − 3 \), \( n_i > 4 \), this means \( i \in A \), to obtain the term \( H_9 \). Finally, we apply Equation 1 to the edges of the cycle \( C_n \) which are \( u_i u_{i+1}, 1 ≤ i ≤ m \), to obtain the terms \( H_{10}, H_{11} \) and \( H_{12} \):

\[
\sum_{i \leq i \leq m} \left( \frac{\delta_{u_i} \delta_{u_{i+1}}}{\delta_{u_i} + \delta_{u_{i+1}}} \right)^3 = H_{10}
\]

\[
\sum_{i \leq i \leq m} \left( \frac{\delta_{u_i} \delta_{u_{i+1}}}{\delta_{u_i} + \delta_{u_{i+1}}} \right)^3 = H_{11}
\]

\[
\sum_{i \leq i \leq m} \left( \frac{\delta_{u_i} \delta_{u_{i+1}}}{\delta_{u_i} + \delta_{u_{i+1}}} \right)^3 = H_{12}
\]

3. Conclusion

In this paper, we computed the Sanskruti index of some chemical trees: caterpillar trees (especially: the tree \( P_n(3, 2, 2, \ldots, 2, 3) \) which is the molecular graph of certain hydrocarbon (straight-chain alkanes)), cycle-caterpillars, starlike trees and sunlike graphs. These results may also hold in other families of molecular graphs. Moreover, there are several research avenues that may naturally extend the results of this paper.

4. References

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