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Research Article

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The Sanskruti index of trees and unicyclic graphs

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Abstract: The Sanskruti index of a graph G is defined as

$$S(G) = \sum_{uv \in E(G)} \left(\frac{s_G(u)s_G(v)}{s_G(u) + s_G(v) - 2} \right)^3,$$

where $s_G(u)$ is the sum of the degrees of the neighbors of a vertex u in G. Let P_n, C_n, S_n and $S_n + e$ be the path, cycle, star and star plus an edge of n vertices, respectively. The Sanskruti index of a molecular graph of a compounds can model the bioactivity of compounds, has a strong correlation with entropy of octane isomers and its prediction power is higher than many existing topological descriptors.

In this paper, we investigate the extremal trees and unicyclic graphs with respect to Sanskruti index. More precisely, we show that

(1) $\frac{512}{27}n - \frac{172688}{3375} \leq S(T) \leq \frac{(n-1)^7}{8(n-2)^3}$ for an n-vertex tree T with $n \geq 3$, with equalities if and only if $T \cong P_n$ (left) and $T \cong S_n$ (right);

(2) $\frac{512}{27}n \leq S(G) \leq \frac{(n-3)(n+1)^3}{8} + \frac{3(n+1)^6}{8n^3}$ for an n-vertex unicyclic graph with $n \geq 4$, with equalities if and only if $G \cong C_n$ (left) and $G \cong S_n + e$ (right).

Keywords: Topological index, Molecular descriptor, Sanskruti index, Tree, Unicyclic graph

Classification: 05C90, 05C05, 92E10

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1 Introduction

In theoretical chemistry, topological indices (or molecular structure descriptors) are utilized as a standard tool to study structure-property relations, especially in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) applications [9, 20]. These topological indices are studied on chemical graphs, whose vertices correspond to the atoms of molecules and edges correspond to chemical bonds [15, 17–19]. In past decades, many topological indices have found important relations between the graph structures and physico-chemical properties [2]. Because of their significant applications, they have been widely studied and applied in many contexts, for example with nanostructures [5, 10], nanomaterials [14], molecular sciences [13], chemistry networks [11], molecular design [1], drug structure analysis [7], fractal graphs [12], and mathematical chemistry [3]. The literature is exhaustive; for example, one of the indices, the Wiener index, along with its applications, is considered in thousands of papers: as of this writing, the seminal paper of Harold Wiener [20] is cited 3535 times according to Google Scholar.

Application of topological indices in biology and chemistry began in 1947 with the work of Harold Wiener [20], who introduced the Wiener index to show correlations between physico-chemical properties of organic compounds and the index of their molecular graphs. This index reveals the correlations of physico-chemical properties of alkanes, alcohols, amines and their analogous compounds [13]. Estrada *et al.* [4] proposed what is now a well-known atom-bond connectivity (ABC) index, which provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes. Inspired by applications of the ABC index, Furtula *et al.* [6] introduced the augmented Zagreb index, whose prediction power was found to be better than that of the ABC index in the study of heat of formation for heptanes and octanes. More recently, Hosamani [10] proposed the Sanskruti index of a molecular graph and showed that it can model the bioactivity of chemical compounds and showed a correlation with entropy of octane isomers that is comparable to or better than some other well-used descriptors. More precisely, according to [10], the model entropy = 1.7857S±81.4286 models the data from dataset found at http://www.moleculardescriptors.eu/dataset.htm with correlation coefficient 0.829 and with standard error 17.837. Soon after, the Sanskruti indices of some graph families of interest in chemical graph theory were established [8, 16].

Motivated by the new proposed Sanskruti index, we investigate the extremal trees and extremal unicyclic graphs with respect to this topological index. Here, we consider only simple graphs, *i.e.*, undirected graphs without loops and multiple edges. Let G be a graph. We denote by $V(G)$ and $E(G)$ the vertex set and edge set of G, respectively. As usual, P_n, C_n, S_n and $S_n + e$ stand for the path, cycle, star and star plus an edge of n vertices, respectively (see Figure 1). We denote by $d_G(v)$ the degree of a vertex v of a graph G and by $N_G(v)$ (or simply $N(v)$) the set of neighbors of v. For two vertices $u, v \in V(G)$, the distance between u and v is the length of a shortest path between u and v. We denote by $N_2(v)$ the set of vertices of distance two from v and by $s_G(u)$ the sum of the degrees of the neighbors of u, *i.e.*, $s_G(u) = \sum_{v\in N_G(u)} d_G(v)$.

Trees are connected graphs without cycles. A vertex in a tree is called a *leaf* if it has degree one, and a vertex is called a *support vertex* if it has a leaf neighbor.

In Section 2, we give some definitions and some preliminary observations. The main results are proved in Section 3: first, we give lower and upper bounds for the Sanskruti index on trees and provide the extremal graphs (Theorems 9 and 10), then we give lower and upper bounds for unicyclic graphs and provide the extremal graphs (Theorems 14 and 15).

2 Preliminaries

The following functions and definitions will be used throughout the paper:

$$f(x, y) = \left(\frac{xy}{x + y - 2}\right)^3. \tag{1}$$

For a graph G and an edge $uv \in E(G)$, we define

$$h(uv|G) = f(s_G(u), s_G(v)) = \left(\frac{s_G(u)s_G(v)}{s_G(u) + s_G(v) - 2}\right)^3, \tag{2}$$

and the Sanskruti index of a graph G is defined as

$$(G) = \sum_{uv\in E(G)} h(uv|G). \tag{3}$$

Based on the above definitions, the following results are immediate, and the proofs are omitted.

Proposition 1 *Let $n \geq 3$, $S(S_n) = \frac{(n-1)^7}{8(n-2)^3}$ and*

$$S(P_n) = \begin{cases} 16, & n = 3, \\ \frac{1753}{64}, & n = 4, \\ \frac{512}{27}n - \frac{172688}{3375}, & n \geq 5. \end{cases}$$

Proposition 2 *Let $n \geq 4$, $S(S_n + e) = \frac{(n-3)(n+1)^3}{8} + \frac{3(n+1)^6}{8n^3}$ and $S(C_n) = \frac{512}{27}n$.*

Lemma 3 *Let $t \geq 3$, $x, y > 0$ and $x + y = t$, then $f(x, y) \leq \frac{t^6}{64(t-2)^3}$. Moreover, $f(x, y) = \frac{t^6}{64(t-2)^3}$ if and only if $x = y = \frac{t}{2}$.*

Lemma 4 *Let $t \neq 2$ and $g(t) = f(\frac{t}{2}, \frac{t}{2}) = \frac{t^6}{64(t-2)^3}$, then $g'(t) = \frac{3(t-4)t^5}{64(t-2)^4}$.*

Lemma 5 *For $x \geq 3$ and $y \geq 3$, f is an increasing function (as a function of one variable, either x or y). In particular, $\frac{\partial f(x,y)}{\partial x} = \frac{3x^2y^3(y-2)}{(x+y-2)^4} \geq 0$and $\frac{\partial f(x,y)}{\partial y} = \frac{3y^2x^3(x-2)}{(x+y-2)^4} \geq 0$.*

The following properties that hold on trees will be useful later.

Lemma 6 *Let T be an n-vertex tree. Then for any edge $uv \in E(T)$, we have*

(a) $N(u) \cap N(v) = \emptyset$ and $N_2(u) \cap N_2(v) = \emptyset$.
(b) $\sum_{v\in N(u)} |N(v)\setminus \{u\}| = |N_2(u)|$.
(c) $s_T(u) = |N_2(u)| + |N(u)| = |N_2(u)| + d_T(u)$ for any $u \in V(T)$.

Proof. (a) Since T contains no C_3, we have $N(u)\cap N(v) = \emptyset$. Suppose to the contrary that $N_2(u)\cap N_2(v) \neq \emptyset$ and let $w \in N_2(u) \cap N_2(v)$. Denote with usw and vtw the shortest $u - w$ path and $v - w$ path. Then $s \neq v$. Otherwise $w \in N(v)$, a contradiction. Analogously, $t \neq u$. Now if $s \neq t$, we obtain that $uvtws$ is a cycle of length five in T, a contradiction. If $s = t$, it follows that uvs is a cycle of length three in T, a contradiction.

(b) From the result of part (a), we have $(N(v_1)\setminus \{u\}) \cap (N(v_2)\setminus \{u\}) = \emptyset$ for any $v_1, v_2 \in N(u)$. Therefore, $\sum_{v\in N(u)} |N(v)\setminus \{u\}| = |N_2(u)|$.

(c) It can be seen that $s_T(u) = \sum_{v\in N(u)} d_T(v) = \sum_{v\in N(u)} |N(v)| = \sum_{v\in N(u)}(|N(v)\setminus \{u\}| + 1) = \sum_{v\in N(u)} |N(v)\setminus \{u\}| + d_T(u)$. From the result of part (b), we have $\sum_{v\in N(u)} |N(v)\setminus \{u\}| = |N_2(u)|$, and thus $s_T(u) = |N_2(u)| + d_T(u)$ for any $u \in V(T)$.

It is obvious that the last property also holds for general graphs without triangles and C_4. We write it as a lemma for later reference.

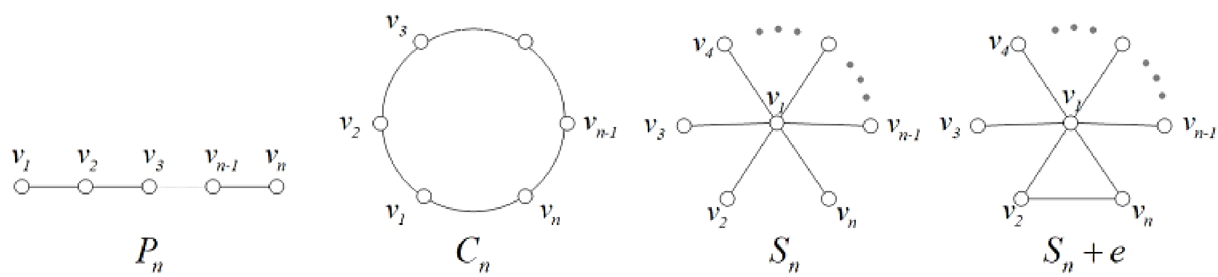

Figure 1: The graphs P_n, C_n, S_n and $S_n + e$

Lemma 7 *Let G be a graph with no triangles and no C_4. Then $s_G(u) = |N_2(u)| + |N(u)| = |N_2(u)| + d_G(u)$ for any $u \in V(G)$.*

In a special case used explicitly in a proof later, we have

Lemma 8 *Let G be an n-vertex unicyclic graph. If G contains a C_4, then for any $u \in V(G)$*

$$s_G(u) = \begin{cases} |N_2(u)| + |N(u)| + 1, & u \in V(C_4), \\ |N_2(u)| + |N(u)|, & u \notin V(C_4). \end{cases}$$

Proof. If $u \in V(C_4)$, we can write $C_4 = uv_1v_2v_3$ and

$$\begin{aligned} s_G(u) &= \sum_{v \in N(u)} |N(v)| \\ &= \sum_{v \in N(u)} |N(v) \setminus \{u\}| + d_G(u) \\ &= \sum_{v \in N(u) \setminus \{v_1, v_3\}} |N(v) \setminus \{u\}| + |N(v_1) \setminus \{u\}| \\ &+ |N(v_3) \setminus \{u\}| + |N(u)| \\ &= |N_2(u)| + 1 + |N(u)|, \end{aligned}$$

because $(N(v_1) \setminus \{u\}) \cap (N(v_3) \setminus \{u\}) = \{v_2\}$.

For $u \notin V(C_4)$, the assertion is obvious. □

3 Main results

3.1 Extremal trees with respect to Sanskruti index

Theorem 9 *Let T be an n-vertex tree with $n \geq 3$. Then, we have*

$$S(T) \leq \frac{(n-1)^7}{8(n-2)^3},$$

with equality if and only if $T \cong S_n$.

Proof. By Lemma 6 (c), we have $s_T(u) + s_T(v) = |N_2(u)| + |N_2(v)| + |N(u)| + |N(v)|$ for any edge $uv \in E(T)$. By Lemma 6 (a), we have $N(u) \cap N(v) = \emptyset$ and $N_2(u) \cap N_2(v) = \emptyset$. Therefore, $s_T(u) + s_T(v) = |N_2(u) \cup N_2(v)| + |N(u) \cup N(v)|$. Since $u, v \notin N_2(u) \cup N_2(v)$, we have $|N_2(u) \cup N_2(v)| \leq n - 2$. It is clear that $|N(u) \cup N(v)| \leq n$, then we have

$$\begin{aligned} s_T(u) + s_T(v) &= |N_2(u) \cup N_2(v)| + |N(u) \cup N(v)| \qquad (4) \\ &\leq 2n - 2. \end{aligned}$$

Moreover,

$$\begin{aligned} s_T(u) + s_T(v) = 2n - 2 &\iff |N_2(u) \cup N_2(v)| \qquad (5) \\ &= n - 2, |N(u) \cup N(v)| = n. \end{aligned}$$

Recall that $f(x, y) = (\frac{xy}{x+y-2})^3$. From Lemmas 3 and 4 it follows that $g(t)$ is an increasing function on the variable t if $t \geq 4$. Note that for any $uv \in E(T)$ with at least three vertices, we have $s_T(u) + s_T(v) \geq 4$, then by applying Lemma 3 with $t = 2n - 2$, we have

$$\begin{aligned} (T) &= \sum_{uv \in E(T)} \left(\frac{s_T(u)s_T(v)}{s_T(u) + s_T(v) - 2} \right)^3 = \sum_{uv \in E(T)} f(s_T(u), s_T(v)) \\ &\leq \sum_{uv \in E(T)} f(x, y)|_{x=y=n-1} = |E(T)| \cdot f(x, y)|_{x=y=n-1} \\ &= \frac{(n-1)^7}{8(n-2)^3}. \end{aligned}$$

Conversely, if $S(T) = \frac{(n-1)^7}{8(n-2)^3}$, then formula (5) holds for any $uv \in E(T)$. It is easy to see that this implies that T must be a star.

Theorem 10 *Let T be an n-vertex tree with $n \geq 3$, then we have*

$$\frac{512}{27} n - \frac{172688}{3375} \leq S(T),$$

with equality if and only if $T \cong P_n$.

Proof. First observe that the lower bound holds for trees with $3 \leq n \leq 6$ vertices (for example, by explicitly comput-

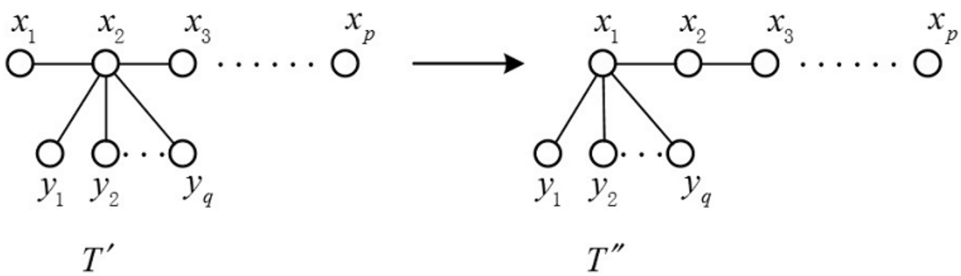

Figure 2: The trees T' and T''

ing the values for all cases). Therefore, we only need to consider the case $n \geq 7$. Let T_n be the family of trees on n vertices and let $F_n = \{T|S(T) \leq S(T'') for any T'' \in T_n, TP_n\}$. Now we need to prove that $F_n = \emptyset$ for any $n \geq 7$.

Suppose to the contrary that there exists an n such that $F_n \neq \emptyset$, and let n be the minimal number with this property. Let $T' \in F_n$ and $P = x_1x_2 \cdots x_p$ be a longest path in T'. Then we claim that

Claim 11. $d(x_2) = 2$.

Proof. If $d(x_2) \geq 3$ write $N(x_2) = \{x_1, x_3, y_1, y_2, \cdots, y_q\}$, where $q \geq 1$. Now construct a new tree T'' with $V(T'') = V(T')$ and $E(T'') = E(T') \cup \{x_1y_i|i = 1, 2, \cdots, q\} \setminus \{x_2y_i|i = 1, 2, \cdots, q\}$ (see Figure 2).

Then we have $s_{T'}(x_3) > s_{T''}(x_3)$ and $s_{T'}(v) \geq s_{T''}(v)$ for any $v \in V(T') \setminus \{x_3\}$. By Lemma 5, and by comparing the contributions of pairs of corresponding edges, we have $S(T') > S(T'')$. Tree T'' thus has a smaller value of Sanskruti index than T', which contradicts the fact that $T' \in F_n$. So, $d(x_2) = 2$.

Claim 12. $d(x_3) = 2$.

Proof. Assume to the contrary that $N(x_3) = \{x_2, x_4, y_1, y_2, \cdots, y_q\}$, where $q \geq 1$. We should consider two cases:

- Case 1: y_1 is a leaf neighbor of x_3.
  Now let $V(T'') = V(T')$ and $E(T'') = E(T') \cup \{x_1y_1\} \setminus \{x_3y_1\}$. Then we have

$$s_{T'}(x_3) > s_{T''}(x_3), \quad s_{T'}(x_2) = s_{T''}(x_2), \tag{6}$$
$$h(x_3y_1|T') = \left(\frac{d_{T'}(x_3)s_{T'}(x_3)}{d_{T'}(x_3) + s_{T'}(x_3) - 2}\right)^3,$$
$$h(x_1x_2|T') = 8, \quad h(x_1y_1|T'') = 8,$$
$$h(x_1x_2|T'') = \left(\frac{3(1 + d_{T'}(x_3))}{d_{T'}(x_3) + 2}\right)^3,$$
$$h(x_2x_3|T'') < h(x_2x_3|T')$$

and

$$h(uv|T'') \leq h(uv|T') \quad for any \quad uv \notin \{x_1x_2, x_1y_1, x_3y_1, x_2x_3\}. \tag{7}$$

Note that $d_{T'}(x_3) \geq 3$ if and only if $\frac{4d_{T'}(x_3)}{d_{T'}(x_3)+2} \geq \frac{3(1+d_{T'}(x_3))}{d_{T'}(x_3)+2}$, thus we have

$$s_{T'}(x_3) \geq 4 \Rightarrow \left(\frac{d_{T'}(x_3)s_{T'}(x_3)}{d_{T'}(x_3) + s_{T'}(x_3) - 2}\right)^3 \geq \left(\frac{3(1 + d_{T'}(x_3))}{d_{T'}(x_3) + 2}\right)^3 \Leftrightarrow h(x_3y_1|T') + h(x_1x_2|T') \geq h(x_1y_1|T'') + h(x_1x_2|T''). \tag{8}$$

From Eqs. (6), (7) and (8) we have that $S(T') > S(T'')$, which is a contradiction. Thus, we have already proved that $d(x_3) = 2$ in case y_1 is a leaf neighbor of x_3.

- Case 2: x_3 has a pendent $P_2 = y_1z_1$.
  Now let $V(T'') = V(T')$ and $E(T'') = E(T') \cup \{x_1y_1\} \setminus \{x_3y_1\}$. Then we have

$$s_{T''}(x_3) = s_{T'}(x_3) - 2,$$
$$d_{T''}(x_3) = d_{T'}(x_3) - 1,$$
$$s_{T''}(x_2) = s_{T'}(x_2),$$
$$s_{T''}(y_1) = 3,$$

and $h(uv|T'') \leq h(uv|T')$ for any $uv \notin \{x_1x_2, x_2x_3, x_3y_1, y_1z_1, x_1y_1\}$. Denote $s_3 = s_{T'}(x_3)$, then $s_3 \geq 5$ and

$$h_1 = h(x_1x_2|T') + h(x_2x_3|T') + h(x_3y_1|T') + h(y_1z_1|T') = 8 + 2\left(\frac{(1 + d_{T'}(x_3))s_3}{d_{T'}(x_3) + s_3 - 1}\right)^3 + 8, \tag{9}$$

$$h_2 = h(x_1x_2|T'') + h(x_2x_3|T'') + h(x_1y_1|T'') + h(y_1z_1|T'') = \left(\frac{4(1 + d_{T'}(x_3))}{3 + d_{T'}(x_3)}\right)^3 + \left(\frac{(1 + d_{T'}(x_3))(s_3 - 2)}{d_{T'}(x_3) + s_3 - 3}\right)^3 + \left(\frac{12}{5}\right)^3 + 8. \tag{10}$$

Define $F(x) = f(x,6) - f(x,4) = \frac{8x^3(x-2)(19x^2+104x+148)}{(x+2)^3(x+4)^3}$. It is obvious that $F(4) = \frac{217}{27}$ and that $F(x)$ is an increasing function for $x \geq 4$.
If $s_3 \geq 6$, since $f(1+d_{T'}(x_3), s_3) - f(1+d_{T'}(x_3), s_3 - 2) \geq 0$, we have

$$\begin{aligned} S(T') - S(T'') &= h_1 - h_2 \geq 8 + f(1+d_{T'}(x_3), 6) \\ &- f(1+d_{T'}(x_3), 4) + f(1+d_{T'}(x_3), s_3) \\ &- f(1+d_{T'}(x_3), s_3 - 2) - \left(\frac{12}{5}\right)^3 = 8 - \left(\frac{12}{5}\right)^3 \\ &+ F(1+d_{T'}(x_3)) + f(1+d_{T'}(x_3), s_3) \\ &- f(1+d_{T'}(x_3), s_3 - 2) \geq 8 - \left(\frac{12}{5}\right)^3 + F(4) = \frac{7469}{3375} \\ &> 0, \end{aligned}$$

a contradiction. It follows $s_3 < 6$. Since $s_3 \geq 5$, it is obvious that $s_3 = 5$. But in this case $d_{T'}(x_4) = 1$. Thus T is isomorphic to a tree with six vertices, which contradicts with $n \geq 7$. So, we have proved that $d(x_3) = 2$ in case x_3 has a pendent $P_2 = y_1 z_1$. Together with Case 1 this means that $d(x_3) = 2$.

Claim 13. $d(x_4) = 2$.

Proof. Suppose to the contrary that $d(x_4) \geq 3$. Let $T'' = T' - \{x_1\}$. By the minimum assumption of n and $T' \in F_n$, we have $S(T'') \geq S(P_{n-1})$. Denote $s_1 = s_{T'}(x_3)$ and $s_2 = s_{T'}(x_4)$, then we have $s_1 \geq 5$ and $s_2 \geq 4$. It can be verified that

$$\left(\frac{3s_1}{s_1+1}\right)^3 + \left(\frac{s_1 s_2}{s_1+s_2-2}\right)^3 + \left(\frac{s_2(s_1-1)}{s_1+s_2-3}\right)^3 > \left(\frac{8}{3}\right)^3. \quad (11)$$

On the other hand, by Proposition 1, we have

$$S(P_n) - S(P_{n-1}) = \left(\frac{8}{3}\right)^3. \quad (12)$$

Therefore, we have

$$\begin{aligned} S(T') &\geq S(T'') + 8 + \left(\frac{3s_1}{s_1+1}\right)^3 + \left(\frac{s_1 s_2}{s_1+s_2-2}\right)^3 - 8 \\ &- \left(\frac{s_2(s_1-1)}{s_1+s_2-3}\right)^3 > S(P_{n-1}) + \left(\frac{3s_1}{s_1+1}\right)^3 \\ &+ \left(\frac{s_1 s_2}{s_1+s_2-2}\right)^3 - \left(\frac{s_2(s_1-1)}{s_1+s_2-3}\right)^3 > S(P_n), \end{aligned}$$

a contradiction. Thus, $d(x_4) = 2$.

Now we have $d_{T'}(x_i) = 2$ for any $i = 2, 3, 4$, and let $T''' = T' - \{x_1\}$. By the minimality assumption on n and $T' \in F_n$, we have $S(T''') > S(P_{n-1})$. Moreover, it can be seen that $S(T''') = S(T') + (\frac{12}{5})^3$. Together with Eq. (12), we have $S(T') > S(P_n)$, a contradiction with minimality of n. Hence $F_n = \emptyset$ for any $n \geq 7$, which completes the proof of Theorem 10.

3.2 Extremal unicyclic graphs with respect to Sanskruti index

Theorem 14 *Let G be an n-vertex unicyclic graph with $n \geq 4$, then we have*

$$S(G) \leq \frac{(n-3)(n+1)^3}{8} + \frac{3(n+1)^6}{8n^3},$$

with equality if and only if $G \cong S_n + e$.

Proof. By Proposition 2, in case $G \cong S_n + e$ we have $S(G) = \frac{(n-3)(n+1)^3}{8} + \frac{3(n+1)^6}{8n^3}$. Now we will show that $S(G) \leq \frac{(n-3)(n+1)^3}{8} + \frac{3(n+1)^6}{8n^3}$ and if $S(G) = \frac{(n-3)(n+1)^3}{8} + \frac{3(n+1)^6}{8n^3}$, then $G \cong S_n + e$.

Suppose to the contrary that $G$is a graph with maximum Sanskruti index, but $GS_n + e$, We consider the following four cases.

- Case 1: Gcontains a C_3.
  Let $C_3 = v_1 v_2 v_3$. Then for any $u \in V(G) \setminus \{v_1, v_2, v_3\}$ we have

$$s_G(u) = |N_2(u)| + |N(u)| \leq n - 1, \quad (13)$$

  and for any $i \in \{1, 2, 3\}$

$$s_G(v_i) = |N_2(v_i)| + |N(v_i)| + 2. \quad (14)$$

  Furthermore, because u_1 and u_2 are not on a cycle, we have for any $u_1 u_2 \notin \{v_1 v_2, v_1 v_3, v_2 v_3\}$

$$s_G(u_1) + s_G(u_2) \leq 2n. \quad (15)$$

  By Eq. (13), it is impossible that $s_G(u_1) = s_G(u_2) = n$. Therefore,

$$h(u_1 u_2 | G) \leq f(n+1, n-1).$$

  Further, we have

$$s_G(v_1) + s_G(v_2) \leq 2n + 2 \quad (16)$$

  and $h(v_1 v_2 | G) \leq f(n+1, n+1)$. It follows

$$\begin{aligned} S(G) &= \sum_{uv \in E(G)} h(uv|G) \\ &\leq 3 f(n+1, n+1) + (n-3) f(n+1, n-1) \\ &= S(S_n + e). \end{aligned}$$

If the equality $S(G) = S(S_n + e)$ holds, then the equalities in (15) and (16) hold and $s_G(v_1) = s_G(v_2) = n + 1$ and $h(u_1u_2|G) = f(n-1, n+1)$ for any $u_1u_2 \notin \{v_1v_2, v_1v_3, v_2v_3\}$. From these results it follows that G is a graph obtained by adding some pendent vertices to a $C_3 = v_1v_2v_3$ and, in addition, all vertices must be attached to the same vertex in $\{v_1, v_2, v_3\}$. Such a graph is isomorphic to $S_n + e$, which is in contradiction with our assumption.

- Case 2: G contains a C_4.
  For any edge uv on the cycle, by Lemma 8, we have

$$s_G(u) \le |N_2(u)| + 1 + |N(u)|, \tag{17}$$

and

$$s_G(v) \le |N_2(v)| + 1 + |N(v)|. \tag{18}$$

Then we have $N_2(u) \cap N_2(v) = \emptyset$, otherwise G contains a C_5. Together with the assumption that G contains C_4 this is a contradiction with the fact that G is unicyclic. Furthermore, we have $N(u) \cap N(v) = \emptyset$. Otherwise G contains a C_3 and this is again a contradiction. Since u and v are not in $N_2(u) \cap N_2(v)$, we have $|N_2(u) \cap N_2(v)| \le n - 2$. As $|N(u) \cap N(v)| \le n$, from Eqs. (17-18) it follows

$$\begin{aligned} s_G(u) + s_G(v) &\le |N_2(u)| + 1 + |N(u)| \\ &+ |N_2(v)| + 1 + |N(v)| \le 2n. \end{aligned} \tag{19}$$

Now we have to consider two separate subcases.

  – Case 2.1: There exists no edge $u'v' \in E(G)$ such that $s_G(u') = s_G(v') = n$.
    In this case, we have $h(uv|G) \le f(n+1, n-1)$ for any edge $uv \in E(G)$. Then

$$\begin{aligned} S(G) &= \sum_{uv \in E(G)} h(uv|G) \\ &\le |E(G)| \cdot f(n+1, n-1) \\ &= n f(n+1, n-1) < 3f(n+1, n+1) \\ &+ (n-3)f(n+1, n-1) = S(S_n + e), \end{aligned}$$

    a contradiction.

  – Case 2.2: There exists an edge $uv \in E(G)$ such that $s_G(u) = s_G(v) = n$.
    Since $u \notin N_2(u) \cup N(u)$ for any $u \in V(G)$, we have $|N_2(u) \cup N(u)| \le n - 1$. Therefore, the equalities hold in Eqs. (17-18) and uv must be in C_4. Then, for any $w \in V(G) - \{u, v\}$, $d(w, v) = 1$ and $d(w, u) = 2$ or $d(w, v) = 2$ and $d(w, u) = 1$. Let $C_4 = uvst$, G is a graph isomorphic to a graph obtained by adding some pendent vertices to u or v of C_4. Then there are at most two edges xy with $s_G(x) = s_G(y) = n$, and hence

$$\begin{aligned} S(G) = \sum_{uv \in E(G)} h(uv|G) &\le 2 f(n, n) \\ &+ (n-2) f(n+1, n-1) < 3 f(n+1, n+1) \\ &+ (n-3) f(n+1, n-1) = S(S_n + e), \end{aligned}$$

    a contradiction.

  From Cases 2.1 and 2.2, it follows that G does not contain C_4.

- Case 3: G contains a C_5.
  By Lemma 7, for any $uv \in E(G)$, we have

$$s_G(u) \le |N_2(u)| + |N(u)|, \tag{20}$$

and

$$s_G(v) \le |N_2(v)| + |N(v)|. \tag{21}$$

  Then $s_G(u) + s_G(v) \le 2n - 1$ and $h(uv|G) \le f(n, n-1)$ for any edge $uv \in E(G)$. It follows

$$\begin{aligned} S(G) = \sum_{uv \in E(G)} h(uv|G) &\le |E(G)| \cdot f(n, n-1) \\ &= nf(n, n-1) < 3f(n+1, n+1) \\ &+ (n-3)f(n+1, n-1) = S(S_n + e), \end{aligned}$$

  a contradiction.

- Case 4: G contains C_k for some $k \ge 6$.
  In this case, for any edge $uv \in E(G)$ we have $s_G(u) + s_G(v) \le 2n - 2$ and $h(uv|G) \le f(n-1, n-1)$. Then

$$\begin{aligned} S(G) &= \sum_{uv \in E(G)} h(uv|G) \\ &\le |E(G)| \cdot f(n-1, n-1) = n \cdot f(n-1, n-1) \\ &< 3 \cdot f(n+1, n+1) + (n-3) \cdot f(n+1, n-1) \\ &= S(S_n + e), \end{aligned}$$

  a contradiction.
  Summing up, we have proved that G does not contain any C_k for all $k \ge 3$, which contradicts the fact that G is an unicyclic graph.

Theorem 15 *Let Gbe an n-vertex unicyclic graph with $n \ge 4$, then we have*

$$\frac{512}{27} n \le S(G),$$

with equality if and only if $G \cong C_n$.

Proof. Suppose G is a graph with minimum Sanskruti index. Let $C = v_1v_2 \cdots v_k$, $3 \le k \le n$, be the unique cycle of G. We consider the following cases.

- Case 1: for any edge v_iv_{i+1} in C we have $s_G(v_i) = 4$ or $s_G(v_{i+1}) = 4$.
  In this case, we have $d(v_j) = 2$ for any v_j in C, and hence $G \cong C$.
  Observe that if $v_i \in C$ and $s_G(v_i) > 4$, then there must be a neighbor of v_i, say $u \in C$ with $s_G(u) > 4$.
- Case 2: there exists an edge v_iv_{i+1} in C such that $s_G(v_i) \geq 5$ and $s_G(v_{i+1}) \geq 5$.

Now we claim that

Claim 16. $s_G(v_i) = 5$ and $s_G(v_{i+1}) = 5$.

Proof. Otherwise, we assume without loss of generality that $s_G(v_{i+1}) \geq 6$. Let $T = G - \{v_iv_{i+1}\}$, then T is a tree. By Theorem 9 we have $S(T) \geq S(P_n)$.

Denote $s_3 = s_G(v_i)$, $s_1 = s_G(v_{i+1})$, $s_2 = s_G(v_{i+2})$.

- ⋆ First, we have $s_3 = 5$. Otherwise, $s_3 \geq 6$. Let $q(x, y) = f(x, y) - f(x-2, y) = (\frac{xy}{x+y-2})^3 - (\frac{(x-2)y}{x+y-4})^3$. Then

$$\frac{\partial q(x,y)}{\partial y} = 3y^2\left(\frac{(x-2)x^3}{(x+y-2)^4} - \frac{(x-4)(x-2)^3)}{(x+y-4)^4}\right) > 0, \tag{22}$$

  which means that function $q(x, y)$ is an increasing function on variable y for fixed $x \geq 4$. Note that $s_2 \geq 4$, so from $s_1 \geq 6$ it follows $q(s_1, s_2) \geq q(s_1, 4)$ and

$$\begin{aligned} S(G) &\geq S(T) + h(v_iv_{i+1}|G) + h(v_{i+1}v_{i+2}|G) \\ &- h(v_{i+1}v_{i+2}|T) \geq S(P_n) + \left(\frac{s_3s_1}{s_3+s_1-2}\right)^3 \\ &+ q(s_1, s_2) \geq S(P_n) + \left(\frac{6s_1}{6+s_1-2}\right)^3 + q(s_1, 4) \\ &> S(C_n), \end{aligned}$$

  contradicting with the assumption that G is a graph with minimum Sanskruti index. Thus, $s_3 = 5$.
- ⋆ Now we have $s_2 \neq 4$. Otherwise, we have $d_G(v_{i+1}) = d_G(v_{i+2}) = 2$, $d_G(v_i) \geq 4$ and thus $s_3 \geq 6$, contradicting with the above result $s_3 = 5$.
- ⋆ Also, we have $s_2 \neq 5$. Otherwise, $s_2 = 5$. Then we have $d_G(v_{i+1}) \leq 3$.
  - If $d_G(v_{i+1}) = 2$, then we have $d_G(v_i) = d_G(v_{i+2}) = 3$ and both v_i and v_{i+2} have a leaf neighbor. Let the leaf neighbor of v_i be v', then we have

$$\begin{aligned} S(G) &\geq S(T) + h(v_iv_{i+1}|G) + h(v_{i+1}v_{i+2}|G) \\ &- h(v_{i+1}v_{i+2}|T) + h(v_iv'|G) - h(v_iv'|T) \\ &\geq S(P_n) + \left(\frac{s_3s_1}{s_3+s_1-2}\right)^3 + q(s_1, s_2) \\ &+ \left(\frac{15}{6}\right)^3 - 8 \geq S(P_n) + \left(\frac{6s_1}{6+s_1-2}\right)^3 \\ &+ q(s_1, 5) + \left(\frac{15}{6}\right)^3 - 8 > S(C_n), \end{aligned}$$

    contradicting with the assumption that G is a graph with minimum Sanskruti index.
  - If $d_G(v_{i+1}) = 3$, then $d_G(v_i) = d_G(v_{i+2}) = 2$. Let $N(v_{i+1}) = \{v_i, v_{i+2}, u'\}$ and $s'_2 = s_G(u')$. Then $s'_2 \geq 4$ and

$$\begin{aligned} S(G) &\geq S(T) + h(v_iv_{i+1}|G) + h(v_{i+1}v_{i+2}|G) \\ &- h(v_{i+1}v_{i+2}|T) + h(v_{i+1}u'|G) - h(v_{i+1}u'|T) \\ &\geq S(P_n) + \left(\frac{s_3s_1}{s_3+s_1-2}\right)^3 + q(s_1, s_2) \\ &+ q(s_1, s'_2) \geq S(P_n) + \left(\frac{s_3s_1}{s_3+s_1-2}\right)^3 \\ &+ q(s_1, 5) + q(s_1, 4) > S(C_n), \end{aligned}$$

    contradicting with the assumption that G is a graph with minimum Sanskruti index.
    Thus, we have proved that $s_2 \neq 5$.
- ⋆ If $s_2 \geq 6$, we exchange the role of v_i and v_{i+2}. Since $s_3 = s_G(v_i) = 5$, we also have $s_2 = s_G(v_{i+2}) = 5$, a contradiction.

Concluding: Claim 16 was proved, we have $s_G(v_i) = 5$ and $s_G(v_{i+1}) = 5$.
Continuing with the proof of Theorem 15 in Case 2 it is sufficient to consider the following two cases.

- Subcase 2.1: $d_G(v_i) = 2$ and $d_G(v_{i+1}) = 2$.
  In this case, obviously $d_G(v_{i-1}) = 3$ and by Claim 16, we have $s_G(v_{i-1}) = 5$, thus v_{i-1} has a leaf neighbor w (see Figure 3 (left)). Let $T = G - \{v_{i-1}v_i\}$, then

$$\begin{aligned} S(G) &\geq S(T) + h(v_{i-1}w|G) - h(v_{i-1}w|T) + h(v_{i-1}v_i|G) \\ &> S(C_n), \end{aligned}$$

  contradicting with the assumption that G is a graph with minimum Sanskruti index.
- Subcase 2.2: $d_G(v_i) = 3$ and $d_G(v_{i+1}) = 2$.
  In this case, v_i has a leaf neighbor w. (see Figure 3 (right)).
  Let $T = G - \{v_iv_{i+1}\}$, then we have

$$\begin{aligned} S(G) &\geq S(T) + h(v_iw|G) - h(v_iw|T) + h(v_iv_{i+1}|G) \\ &> S(C_n), \end{aligned}$$

  contradicting with the assumption that $G$is a graph with minimum Sanskruti index.

This concludes the proof of Theorem 15.

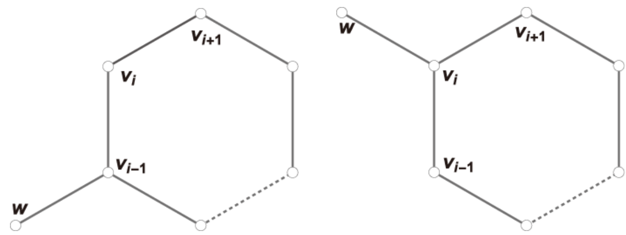

Figure 3: The case $d_G(v_i) = 2$ and $d_G(v_{i+1}) = 2$ (left); the case $d_G(v_i) = 3$ and $d_G(v_{i+1}) = 2$ (right).

4 Conclusions and future work

This paper reveals the idea that the structure of a molecular tree or unicyclic graph with minimal Sanskruti index has a path as long as possible. Similarly, a tree or a unicyclic graph with maximal value of Sanskruti index has a path as short as possible, 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. A natural generalization of trees and unicyclic graphs are cactus graphs, and it may be possible to find the extremal graphs among cacti applying the methods used here. Another idea that may be worth investigation is the following: the exponent 3 in the definition of Sanskruti index seems to be a rather arbitrary and lucky choice. One could replace 3 with arbitrary exponent $\alpha > 0$ and perhaps obtain similar mathematical properties, and for some other α maybe even better correlation with some chemical properties of the corresponding chemical graphs.

Ethical approval: The conducted research is not related to either human or animal use.

Conflict of interest: Authors state no conflict of interest.

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