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The Maximum Hosoya Index of Unicyclic Graphs with Diameter at Most Four

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Abstract: The Hosoya index of a graph is defined by the total number of the matchings of the graph. In this paper, we determine the maximum Hosoya index of unicyclic graphs with n vertices and diameter 3 or 4. Our results somewhat answer a question proposed by Wagner and Gutman in 2010 for unicyclic graphs with small diameter.

Keywords: Hosoya index; unicyclic graphs; diameter

1. Introduction

Numerous topological and chemical indices/measures have been used for analyzing molecular graphs [1–4]. A prominent example is the Hosoya index introduced by Hosoya [5] in 1971 as a molecular-graph based structure descriptor. Hosoya discovered that certain physico-chemical properties of alkanes (= saturated hydrocarbons)—in particular, their boiling points—are well correlated with this index. Gutman et al. further considered it in the chemical view [6]. As is known, structural graph descriptors have been investigated extensively in chemistry, drug design and related disciplines [1–4].

The Hosoya index got much attention by many researchers in the past decades. They have been interested in identifying the maximum or minimum value of Hosoya index for various classes of graphs (with certain restrictions), such as trees [7–9], unicyclic graphs [10–14], bicyclic graphs [15] and so on. For an exhaustive survey for this topic, we refer to [16].

Even though there is a considerable amount of literature on the topic of maximizing or minimizing the Hosoya index, there are still many interesting open questions left. In [16], it is mentioned that:

- *It seems to be difficult to obtain results of the maximum Hosoya index among trees with a given number of leaves or given diameter. However, partial results are available, so the problem might not be totally intractable, and results in this direction would definitely be interesting.*
- *If the aforementioned questions can be answered for trees, then it is also natural to consider the analogous questions for treelike graphs (such as unicyclic graphs).*

For two vertices u, v in a graph G, the distance $d(u, v)$ between u and v is the length of a shortest path connecting them. The diameter of G is $\max\{d(u, v) \mid u, v \in V(G)\}$. Confirming a conjecture proposed by Ou [12], Liu [8] considered the maximum Hosoya index of trees with diameter 4. Motivated by this line of research, we here consider the maximal Hosoya index of unicyclic graphs with small diameter. It seems that unicyclic graphs are only one more edge than trees, however, some of their properties change drastically such as the girth.

At the end of this section, we define some notation as well as some preliminary results that we frequently use in the sequel.

Let G be a simple connected graph with vertex set $V(G)$. For $u \in V(G)$, we denote its neighborhood by $N_G(u)$, and denote $d_G(u) := N_G(u)$. A pendent vertex is a vertex of degree 1. For two vertices u_1 and u_2, the distance between u_1 and u_2 is the number of edges in a shortest path joining u_1 and u_2. We use $G - u$ to denote the graph that arises from G by deleting the vertex $u \in V(G)$. For other undefined notations, we refer to [17].

Given a molecular graph G, let $m(G,k)$ be the number of k matchings of G. It would be convenient to define $m(G,0) = 1$, $m(G,1) = e(G)$. The Hosoya index $z = z(G)$ is defined as the number of subsets of $E(G)$ in which no edges are incident, in other words, the total number of the matchings of the graph G. Then,

$$z(G) = \sum_{k \geq 0} m(G,k).$$

For the star $K_{1,p}$ of order $p+1$, when $k \geq 2$, we have $m(G,k) = 0$. Then, $z(K_{1,p}) = \sum_{k\geq 0} m(G,k) = m(G,0) + m(G,1) = 1 + p$.

The double star $S_{p,q}$ is a tree of order n obtained from $K_{1,p}$ and $K_{1,q-1}$, by identifying a pendent vertex of $K_{1,p}$ with the center of $K_{1,q-1}$, where $p + q = n$. For $S_{p,q}$, when $k \geq 3$, we have $m(G,k) = 0$, therefore

$$\begin{aligned} z(S_{p,q}) &= \sum_{k \geq 0} m(G,k) = m(G,0) + m(G,1) + m(G,2) \\ &= 1 + (p+q-1) + (p-1)(q-1) = pq + 1. \end{aligned}$$

The following two lemmas are needed in this paper, which can be found on page 337 of [16].

Lemma 1. *Let G be a graph and v be a vertex of G. Then,*

$$z(G) = z(G - v) + \sum_{u \in N_G(v)} z(G - \{u, v\}).$$

Lemma 2. *If $G_1, G_2, \ldots, G_t$ are the components of a graph G, then*

$$z(G) = \Pi_{i=1}^{t} z(G_i).$$

For $n \geq 6$, the unique unicyclic graph with diameter two is obtained from the star $K_{1,n-1}$ by adding an edge. For unicyclic graphs with diameter at least 5, things become more complicated, and we believe more techniques are needed. Thus, we only consider the cases for diameter 3 and 4. In Section 2, we determine the maximal Hosoya index of unicyclic graphs with n vertices and diameter 3 (see Theorem 5). In Section 3, we determine the maximal Hosoya index of unicyclic graphs with n vertices and diameter 4 (see Theorem 15).

2. The Unicyclic Graphs with Diameter 3

In this section, we study the maximal Hosoya index of unicyclic graphs with n vertices and diameter 3.

Let $\mathcal{U}_n^3$ be the set of all unicyclic graphs with n vertices and diameter 3. According to the length of the unique cycle and the distribution of other vertices, we may classify all the members in $\mathcal{U}_n^3$. Let $\mathcal{U}_i$

be the set of unicyclic graph of the form G_i, $i = 1, 2, 3, 4$. It is easy to see that the graphs from $\mathcal{U}_1, \mathcal{U}_2$, $\mathcal{U}_3$, and $\mathcal{U}_4$, and C_5, C_6, and C_7 are all unicyclic graphs with diameter 3.

Let $\mathcal{U}_1$ be the set of unicyclic graphs of the form G_1 (as depicted in Figure 1), where $a + b + c = n$, $a, b, c \geq 1$ and at least two of a, b, c are greater than 2. Let G_1^* be the graph of the form G_1 satisfying a, b, c almost equal (hereafter "almost equal" means the difference of any two numbers is at most one).

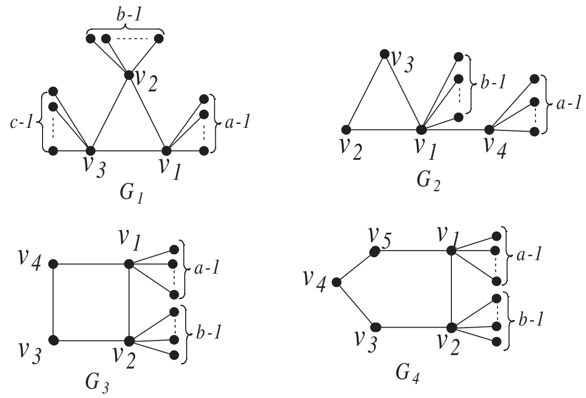

Figure 1. Four unicyclic graphs with diameter 3.

Theorem 1. *The graph G_1^* has the maximum Hosoya index among all graphs in $\mathcal{U}_1$.*

Proof. Assume $G_1 \in \mathcal{U}_1$ with $1 \leq a \leq b \leq c$. By Lemmas 1 and 2, we obtain

$$\begin{aligned}
z(G_1) &= z(G_1 - v_1) + \sum_{w \in N_{G_1}(v_1)} z(G_1 - \{v_1, w\}) \\
&= z(G_1 - v_1) + z(G_1 - \{v_1, v_2\}) + z(G_1 - \{v_1, v_3\}) \\
&+ (a-1) z(G_1 - \{v_1, y\}) \\
&= (bc + 1) + c + b + (a-1)(bc+1) \\
&= abc + a + b + c := f_1(a, b, c),
\end{aligned}$$

where y is one of pendent vertex adjacent to v_1 in G_1.

If $b - a \geq 2$, then we get

$$f_1(a+1, b-1, c) - f_1(a, b, c) = (b - a - 1)c > 0.$$

As a, b, c have the same status as shown in the graph, we conclude that, when a, b, c are almost equal, G_1 has the maximal Hosoya index. □

Let $\mathcal{U}_2$ be the set of unicyclic graphs of the form G_2 (as depicted in Figure 1), where $a + b = n - 2$, $a \geq 2, b \geq 1$. Let G_2^* be the graph of the form G_2 satisfying $0 \leq a - b \leq 2$.

Theorem 2. *The graph G_2^* has the maximum Hosoya index among all graphs in $\mathcal{U}_2$.*

Proof. Assume $G_2 \in \mathcal{U}_2$. By Lemmas 1 and 2, we obtain

$$\begin{aligned}
z(G_2) &= z(G_2 - v_1) + \sum_{v' \in N_{G_2}(v_1)} z(G_2 - \{v_1, v'\}) \\
&= z(G_2 - v_1) + z(G_2 - \{v_1, v_2\}) + z(G_2 - \{v_1, v_3\}) \\
&+ z(G_2 - \{v_1, v_4\}) + (b-1) z(G_2 - \{v_1, y\}) \\
&= 2a + a + a + 2 + 2a(b-1) \\
&= 2ab + 2a + 2 := f_2(a, b),
\end{aligned}$$

where y is one of pendent vertexs adjacent to v_1 in G_2.

If $b - a \geq 1$, then we get

$$f_2(a+1, b-1) - f_2(a, b) = 2(b-a) > 0.$$

If $a - b \geq 3$, then we get

$$f_2(a-1, b+1) - f_2(a, b) = 2(a-b-2) > 0.$$

Thus, we obtain the result. □

Let $\mathcal{U}_3$ be the set of unicyclic graph of the form G_3 (as depicted in Figure 1), where v_1 and v_2 are two vertices with $a-1$, $b-1$ pendent vertices satisfying $a+b = n-2, a, b \geq 1$, one of a and b is at least 2. Let G_3^* be the graph of the form G_3 satisfying a, b almost equal.

Theorem 3. *The graph G_3^* has the maximum Hosoya index among all graphs in $\mathcal{U}_3$.*

Proof. For $G_3 \in \mathcal{U}_3$ with $a \geq b \geq 1$, by Lemmas 1 and 2, we obtain

$$\begin{aligned} z(G_3) &= z(G_3 - v_1) + \sum_{v' \in N_{G_3}(v_1)} z(G_3 - \{v_1, v'\}) \\ &= z(G_3 - v_1) + z(G_3 - \{v_1, v_2\}) + z(G_3 - \{v_1, v_4\}) \\ &+ (a-1) z(G_3 - \{v_1, y\}) \\ &= (2b+1) + 2 + (b+1) + (a-1)(2b+1) \\ &= 2ab + a + b + 3 := f_3(a, b), \end{aligned}$$

where y is one of pendent vertex adjacent to v_1 in G_3.

If $a - b \geq 2$, then we get

$$f_3(a-1, b+1) - f_3(a, b) = 2(a-b-1) > 0.$$

Therefore, when a and b are almost equal, G_2 has the maximal Hosoya index. □

Let $\mathcal{U}_4$ be the set of unicyclic graphs of the form G_4 (as depicted in Figure 1), where v_1 and v_2 are two vertices with $a-1$, $b-1$ pendent vertices, respectively, $a+b = n-3$, $a, b \geq 1$. Let G_4^* be the graph of the form G_4 satisfying $|a-b| \leq 1$.

Theorem 4. *The graph G_4^* has the maximum Hosoya index among all graphs in $\mathcal{U}_4$.*

Proof. Assume $G_4 \in \mathcal{U}_4$ with $a \geq 2, b \geq 1$. By Lemmas 1 and 2, we obtain

$$\begin{aligned}
z(G_4) &= z(G_4 - v_1) + \sum_{v' \in N_{G_4}(v_1)} z(G_4 - \{v_1, v'\}) \\
&= z(G_4 - v_1 - v_2) + \sum_{y \in N_{G_4 - v_1}(v_2)} z(G_4 - v_1 - \{v_2, y\}) \\
&+ \sum_{v' \in N_{G_4}(v_1)} z(G_4 - \{v_1, v'\}) \\
&= z(G_4 - v_1 - v_2) + [z(G_4 - v_1 - \{v_2, v_3\}) \\
&+ (b-1) z(G_4 - v_1 - \{v_2, y\})] \\
&+ [z(G_4 - \{v_1, v_2\}) + z(G_4 - \{v_1, v_5\}) \\
&+ (a-1) z(G_4 - \{v_1, v'\})] \\
&= [3 + 2 + 3(b-1)] + [3 + 2b + 1 + (a-1)(3b+2)] \\
&= 3ab + 2a + 2b + 4 := f_4(a, b),
\end{aligned}$$

where v' is a pendent vertex adjacent to v_1, y is a pendent vertex adjacent to v_2.

If $a - b \geq 2$, then we get

$$f_4(a-1, b+1) - f_4(a, b) = 3(a - b - 1) > 0.$$

This implies the result. □

Theorem 5. *The graph G_1^* has the maximum Hosoya index among all graphs in $\mathcal{U}_n^3$ if $n \geq 17$.*

Proof. We only need to compare the Hosoya indices of G_i^* for $i = 1, 2, 3, 4$.

For G_1^*, we assume that $a \leq b \leq c$. As a, b, c are almost equal and $a + b + c = n$, then we have $a \geq \frac{n-2}{3}$. Thus,

$$\begin{aligned}
z(G_1^*) &= abc + a + b + c \\
&\geq \frac{(n-2)^3}{27} + n := g_1(n).
\end{aligned}$$

For G_2^*, as $0 \leq a - b \leq 2$ and $a + b = n - 2$, we have $a - 2 \leq b \leq a$ and thus $a \leq \frac{n}{2}$. Thus

$$\begin{aligned}
z(G_2^*) &= 2ab + 2a + 2 \\
&\leq 2a^2 + 2a + 2 \\
&\leq \frac{n^2}{2} + n + 2 := g_2(n).
\end{aligned}$$

The last inequality holds for a function $f(a) = 2a^2 + 2a + 2$ that is strictly increasing for $1 \leq a \leq \frac{n}{2}$.

For G_3^*, as a, b are almost equal and $a + b = n - 2$, then we have

$$\begin{aligned}
z(G_3^*) &= 2ab + a + b + 3 \\
&\leq \frac{(a+b)^2}{2} + a + b + 3 \\
&= \frac{(n-2)^2}{2} + n + 1 := g_3(n).
\end{aligned}$$

For G_4^*, as a, b are almost equal and $a+b=n-3$, then we have

$$\begin{aligned} z(G_4^*) &= 3ab+2a+2b+4 \\ &\leq \frac{3(a+b)^2}{4}+2(a+b)+4 \\ &= \frac{3(n-3)^2}{4}+2n-2 := g_4(n). \end{aligned}$$

By using the software "Mathematica", we see $g_4(n) > g_2(n) > g_3(n)$ for $n \geq 14$, $g_1(n) > g_4(n)$ for $n \geq 17$. A direct computation yields to $z(C_5) = 11, z(C_6) = 18, z(C_7) = 29$.

From above, we obtain the result. □

3. The Unicyclic Graphs with Diameter 4

In this section, we aim to determine the maximal Hosoya index of unicyclic graphs with n vertices and diameter 4.

Let $\mathcal{V}_n^4$ be the set of all unicyclic graphs with n vertices and diameter 4. According to the length of the unique cycle and the distribution of other vertices, we may classify all the members in $\mathcal{V}_n^4$. Let $\mathcal{V}_i$ be the set of unicyclic graphs of the form H_i, $i = 1,2,3,4,5,6,7,8$. It is easy to see that the graphs from $\mathcal{V}_1$, $\mathcal{V}_2$, $\mathcal{V}_3$, $\mathcal{V}_4$, $\mathcal{V}_5$, $\mathcal{V}_6$, $\mathcal{V}_7$, $\mathcal{V}_8$, and $\mathcal{V}_9$ and two cycles C_8 and C_9 are all members of the unicyclic graphs with diameter 4.

Let $\mathcal{V}_1$ be the set of unicyclic graphs of the form H_1 (as depicted in Figure 2), where v_1, v_4, and v_5 are three vertices with $c-1$, $b-1$, and $a-1$ pendent vertices, $a+b+c = n-2$, $a \geq 2, b \geq 1, c \geq 1$. Let H_1^* be the graph of the form H_1 satisfying $0 \leq a-b \leq 1, 0 \leq a-c \leq 2, 0 \leq b-c \leq 1$.

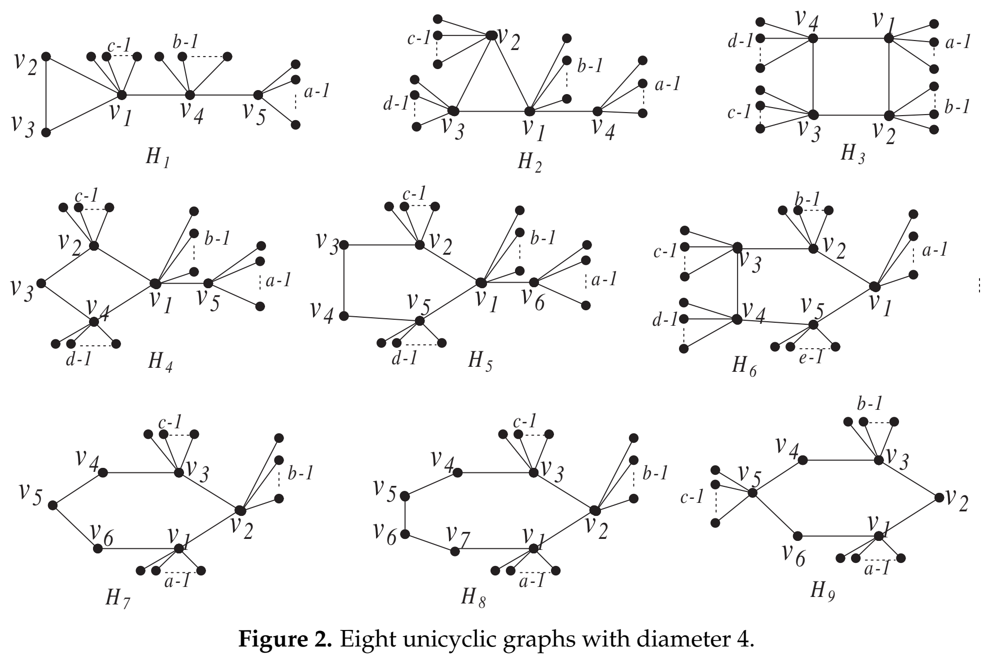

Figure 2. Eight unicyclic graphs with diameter 4.

Theorem 6. *The graph H_1^* has the maximum Hosoya index among all graphs in $\mathcal{V}_1$.*

Proof. For $H_1 \in \mathcal{V}_1$, by Lemmas 1 and 2, we have

$$\begin{aligned} z(H_1) &= z(H_1 - v_1) + \sum_{v' \in N_{H_1}(v_1)} z(H_1 - \{v_1, v'\}) \\ &= z(H_1 - v_1) + z(H_1 - \{v_1, v_2\}) + z(H_1 - \{v_1, v_3\}) \\ &+ z(H_1 - \{v_1, v_4\}) + (c-1) z(H_1 - \{v_1, y\}) \\ &= 2(ab+1) + (ab+1) + (ab+1) + 2a + 2(c-1)(ab+1) \\ &= 2abc + 2ab + 2a + 2c + 2 := g_1(a,b,c), \end{aligned}$$

where y is one pendent vertex adjacent to v_1 in H_1.

Case 1. If $b - a \geq 1$, then

$$g_1(a+1, b-1, c) - g_1(a,b,c) = (b-a-1)(2c+2) + 2 > 0.$$

Case 2. If $a - b \geq 2$, then

$$g_1(a-1, b+1, c) - g_1(a,b,c) = (a-b-1)(2c+2) - 2 \geq 2c > 0.$$

Cases 1 and 2 imply that, if H_1 has maximum Hosoya index, then we infer $0 \leq a - b \leq 1$.

Case 3. If $c - a \geq 1$, then

$$g_1(a+1, b, c-1) - g_1(a,b,c) = 2b(c-a-1) + 2b > 0.$$

Case 4. If $a - c \geq 3$, then

$$g_1(a-1, b, c+1) - g_1(a,b,c) = 2b(a-c-2) \geq 2b > 0.$$

Cases 3 and 4 imply that, if H_1 has maximum Hosoya index, then we infer $0 \leq a - c \leq 2$.

Case 5. If $c - b \geq 1$, then

$$g_1(a, b+1, c-1) - g_1(a,b,c) = 2a(c-b) - 2 > 0.$$

Case 6. If $b - c \geq 2$, then

$$g_1(a, b-1, c+1) - g_1(a,b,c) = 2a(b-c-2) + 2 > 0.$$

Cases 5 and 6 imply that if H_1 has maximum Hosoya index, then we infer $0 \leq b - c \leq 1$ are almost equal.

From the above, we get the result. □

Let $\mathcal{V}_2$ be the set of unicyclic graphs of the form H_2 (as depicted in Figure 2), where v_4, v_1, v_2, and v_3 are four vertices with $a-1$, $b-1$, $c-1$, and $d-1$ pendent vertices, respectively, $a+b+c+d = n$. As the diameter is 4, we infer $a \geq 2$ and one value of c and d is at least 2. Let H_2^* be the graph of the form H_2 satisfying $0 \leq a - b \leq 2$, $0 \leq a - c \leq 1$, $|c - d| \leq 1$.

Theorem 7. *The graph H_2^* has the maximum Hosoya index among all graphs in $\mathcal{V}_2$.*

Proof. For $H_2 \in \mathcal{V}_2$, by Lemmas 1 and 2, we have

$$\begin{aligned} z(H_2) &= z(H_2 - v_1) + \sum_{v' \in N_{H_2}(v_1)} z(H_2 - \{v_1, v'\}) \\ &= z(H_2 - v_1) + z(H_2 - \{v_1, v_2\}) + z(H_2 - \{v_1, v_3\}) \\ &+ z(H_2 - \{v_1, v_4\}) + (b-1)z(H_2 - \{v_1, y\}) \\ &= a(cd+1) + ad + ac + (cd+1) + a(b-1)(cd+1) \\ &= abcd + ab + ac + ad + cd + 1 := g_2(a,b,c,d), \end{aligned}$$

where y is one of pendent vertex adjacent to v_1 in H_2.

Case 1. If $c - d \geq 2$, then

$$g_2(a,b,c-1,d+1) - g_2(a,b,c,d) = (ab+1)(c-d-1) > 0.$$

Case 2. If $d - c \geq 2$, we infer

$$g_2(a,b,c+1,d-1) - g_2(a,b,c,d) = (ab+1)(d-c-1) > 0.$$

Cases 1 and 2 imply that, if H_2 has maximum Hosoya index, then we infer $|c-d| \leq 1$.

Case 3. If $a - b \geq 3$, then

$$\begin{aligned} g_2(a-1,b+1,c,d) - g_2(a,b,c,d) &= (a-b-1)cd \\ &+ (a-b-1) - c - d \\ &\geq 2cd + 2 - c - d \\ &= cd + 1 + (c-1)(d-1) > 0. \end{aligned}$$

Case 4. If $b - a \geq 1$, then

$$\begin{aligned} g_2(a+1,b-1,c,d) - g_2(a,b,c,d) &= (b-a-1)cd \\ &+ (b-a-1) + c + d \\ &\geq c + d > 0. \end{aligned}$$

Cases 3 and 4 imply that, if H_2 has maximum Hosoya index, then infer $0 \leq a - b \leq 2$.

Case 5. If $a - c \geq 2$, then

$$\begin{aligned} g_2(a-1,b,c+1,d) - g_2(a,b,c,d) &= (a-c-1)bd \\ &- b + (a-c-1) \\ &\geq bd - b + 1 > 0. \end{aligned}$$

Case 6. If $c - a \geq 1$, then

$$\begin{aligned} g_2(a+1,b,c-1,d) - g_2(a,b,c,d) &= (c-a-1)bd \\ &+ b + (c-a-1) \\ &\geq b > 0. \end{aligned}$$

Cases 5 and 6 imply that, if H_2 has maximum Hosoya index, then we infer $0 \leq a - c \leq 1$.

From the above cases, we get the result. □

Let $\mathcal{V}_3$ be the set of unicyclic graphs of the form H_3 (as depicted in Figure 2), where v_1, v_2, v_3, and v_4 are four vertices with $a-1$, $b-1$, $c-1$, and $d-1$ pendent vertices, $a+b+c+d = n$, $a,b,c,d \geq 1$.

As the diameter is 4, a and c, or b and d, are at least 2. Let H_3^* be the graph of the form H_3 satisfying a,b,c,d almost equal.

Theorem 8. *The graph H_3^* has the maximum Hosoya index among all graphs in $\mathcal{V}_3$.*

Proof. For $H_3 \in \mathcal{V}_3$, by Lemmas 1 and 2, we have

$$z(H_3) = z(H_3 - v_1) + \sum_{v' \in N_{H_3}(v_1)} z(H_3 - \{v_1, v'\}).$$

For $z(H_3 - v_1)$, by Lemma 1, we have

$$\begin{aligned} z(H_3 - v_1) &= z(H_3 - v_1 - v_2) + \sum_{v' \in N_{H_3 - v_1}(v_2)} z(H_3 - v_1 - \{v_2, v'\}) \\ &= z(H_3 - v_1 - v_2) \\ &\quad + z(H_3 - v_1 - \{v_2, v_3\}) \\ &\quad + (b-1) z(H_3 - v_1 - \{v_2, y\}) \\ &= (cd+1) + d + (b-1)(cd+1) \\ &= bcd + b + d, \end{aligned}$$

where y is one pendent vertex adjacent to v_2 in H_3.

For $\sum_{v' \in N_{H_3}(v_1)} z(H_3 - \{v_1, v'\})$, by Lemmas 1 and 2, we have

$$\begin{aligned} &\sum_{v' \in N_{H_3}(v_1)} z(H_3 - \{v_1, v'\}) \\ &= z(H_3 - \{v_1, v_2\}) + z(H_3 - \{v_1, v_4\}) + (a-1) z(H_3 - \{v_1, w\}) \\ &= (cd+1) + (bc+1) + (a-1)(bcd + b + d), \end{aligned}$$

where w is one of pendent vertex adjacent to v_1 in H_3. Therefore,

$$\begin{aligned} z(H_3) &= z(H_3 - v_1) + \sum_{v' \in N_{H_3}(v_1)} z(H_3 - \{v_1, v'\}) \\ &= (bcd + b + d) + [(cd+1) + (bc+1) + (a-1)(bcd + b + d)] \\ &= abcd + ab + ad + bc + cd + 2 := g_3(a,b,c,d). \end{aligned}$$

Case 1. If $a - c \geq 2$, then

$$g_3(a-1, b, c+1, d) - g_3(a,b,c,d) = bd(a-c-1) > 0.$$

From Case 1, we have, when a and c are almost equal, H_3 has larger Hosoya index. Similarly, as b, d have the same status as shown in the graph, we conclude that, when b and d are almost equal, H_3 has larger Hosoya index.

Case 2. If $a - b \geq 2$, then

$$\begin{aligned} g_3(a-1, b+1, c, d) - g_3(a,b,c,d) &= (a-b-1)cd \\ &\quad + (a-b-1) - d + c \\ &\geq cd + 1 - d + c \\ &= (c-1)(d+1) + 2 > 0. \end{aligned}$$

Therefore, from Case 2, when H_3 has maximum Hosoya index, we infer that a and b are almost equal, and, similarly, a and d are almost equal.

From Case 1, b and d are almost equal, so a, b and d are almost equal. Similarly, a, b and c are almost equal. Hence, we get a, b, c, d are almost equal. □

Let $\mathcal{V}_4$ be the set of unicyclic graphs of the form H_4 (as depicted in Figure 2), where v_5, v_1, v_2, and v_4 are four vertices with $a-1$, $b-1$, $c-1$, and $d-1$ pendent vertices with $a+b+c+d=n$, $a \geq 2, b, c, d \ \geq 1$. Let H_4^* be the graph of the form H_4 satisfying $0 \leq a-b \leq 2, |c-d| \leq 1, 0 \leq a-c \leq 1$.

Theorem 9. *The graph H_4^* has the maximum Hosoya index among all graphs in $\mathcal{V}_4$.*

Proof. For $H_4 \in \mathcal{V}_4$, by Lemmas 1 and 2, we have

$$z(H_4) = z(H_4 - v_1) + \sum_{v' \in N_{H_4}(v_1)} z(H_4 - \{v_1, v'\}).$$

For $z(H_4 - v_1)$, by Lemma 1, we get

$$\begin{aligned} z(H_4 - v_1) &= z(H_4 - v_1 - v_2) + \sum_{v' \in N_{H_4 - v_1}(v_2)} z(H_4 - v_1 - \{v_2, v'\}) \\ &= z(H_4 - v_1 - v_2) + z(H_4 - v_1 - \{v_2, v_3\}) \\ &+ (c-1) z(H_4 - v_1 - \{v_2, y\}) \\ &= a(d+1) + ad + (c-1)a(d+1) \\ &= acd + ac + ad, \end{aligned}$$

where y is one pendent vertex adjacent to v_2 in H_4. For $\sum_{v' \in N_{H_4}(v_1)} z(H_4 - \{v_1, v'\})$, by Lemmas 1 and 2,

$$\begin{aligned} \sum_{v' \in N_{H_4}(v_1)} z(H_4 - \{v_1, v'\}) &= z(H_4 - \{v_1, v_2\}) + z(H_4 - \{v_1, v_4\}) \\ &+ z(H_4 - \{v_1, v_5\}) \\ &+ (b-1) z(H_4 - \{v_1, v_{b-1}\}) \\ &= z(H_4 - \{v_1, v_2\}) \\ &+ z(H_4 - \{v_1, v_4\}) \\ &+ [z(H_4 - \{v_1, v_5\} - v_2) \\ &+ z(H_4 - \{v_1, v_5\} - \{v_2, v_3\}) \\ &+ (c-1) z(H_4 - \{v_1, v_5\} - \{v_2, y\})] \\ &+ (b-1) z(H_4 - \{v_1, w\}) \\ &= a(d+1) + a(c+1) \\ &+ (cd + c + d) \\ &+ (b-1)(acd + ac + ad), \end{aligned}$$

where w is one pendent vertex adjacent to v_1 in H_4. Hence, it follows that

$$\begin{aligned}z(H_4) &= z(H_4 - v_1) + \sum_{v' \in N_{H_4}(v_1)} z(H_4 - \{v_1, v'\}) \\ &= (acd + ac + ad) \\ &+ [a(d+1) + a(c+1) \\ &+ (cd + c + d) + (b-1)(acd + ac + ad)] \\ &= abcd + abc + abd + ac + ad + cd + 2a + c + d \\ &:= g_4(a,b,c,d).\end{aligned}$$

Case 1. If $c - d \geq 2$, then

$$\begin{aligned}g_4(a,b,c-1,d+1) - g_4(a,b,c,d) - (abcd + abc \\ + abd + ac + ad \\ + cd + 2a + c + d) \\ = (ab+1)(c-d-1) > 0.\end{aligned}$$

Similarly, if $d - c \geq 2$, then we have

$$g_4(a,b,c+1,d-1) - g_4(a,b,c,d) = (ab+1)(d-c-1) > 0.$$

Cases 1 implies that, if H_4 has the maximum Hosoya index, we conclude $|d - c| \leq 1$.
Case 2. If $a - b \geq 3$, then

$$\begin{aligned}g_4(a-1,b+1,c,d) - g_4(a,b,c,d) &= (a-b-1)cd \\ &+ (a-b-1)(c+d) \\ &- c - d - 2 \\ &\geq 2cd + c + d - 2 > 0.\end{aligned}$$

Case 3. If $b - a \geq 1$, then

$$\begin{aligned}&g_4(a+1,b-1,c,d) - g_4(a,b,c,d) \\ &= (b-a-1)cd + (b-a-1)(c+d) + c + d + 2 \\ &\geq c + d + 2 > 0.\end{aligned}$$

Cases 2 and 3 imply that, if H_4 has the maximum Hosoya index, we conclude $0 \leq a - b \leq 2$.
Case 4. If $a - c \geq 2$, then

$$\begin{aligned}g_4(a-1,b,c+1,d) - g_4(a,b,c,d) &= (a-c-1)bd \\ &+ (a-c-1)b \\ &- bd + (a-c-1) - 1 > 0.\end{aligned}$$

.

Case 5. If $c - a \geq 1$, then

$$\begin{aligned}g_4(a+1,b,c-1,d) - g_4(a,b,c,d) &= (c-a-1)bd \\ &+ (c-a-1)b + bd \\ &+ (c-a-1) + 1 > 0.\end{aligned}$$

Thus, we have $z(H_{46}) > z(H_4)$.
Cases 4 and 5 imply that, if H_4 has the maximum Hosoya index, we conclude $0 \leq a - c \leq 1$.
All the above cases imply the desired result. □

Let $\mathcal{V}_5$ be the set of unicyclic graphs of the form H_5 (as depicted in Figure 2), where v_6, v_1, v_2, and v_5 are four vertices with $a-1$, $b-1$, $c-1$, and $d-1$ pendent vertices, $a+b+c+d=n-2$, and $a\geq 2, b, c, d \ \geq 1$. Let H_5^* be the graph of the form H_5 satisfying $0\leq a-b\leq 2, |c-d|\leq 1, 0\leq a-c\leq 1$.

Theorem 10. *The graph H_5^* has the maximum Hosoya index among all graphs in $\mathcal{V}_5$.*

Proof. For $H_5\in\mathcal{V}_5$, by Lemmas 1 and 2,

$$\begin{aligned}z(H_5) &= z(H_5-v_1)+\sum_{v'\in N_{H_5}(v_1)} z(H_5-\{v_1,v'\})\\ &= z(H_5-v_1)+z(H_5-\{v_1,v_2\})+z(H_5-\{v_1,v_5\})\\ &+z(H_5-\{v_1,v_6\})+(b-1)z(H_5-\{v_1,y\}),\end{aligned}$$

where y is one pendent vertex adjacent to v_1 in H_5.

For $z(H_5-v_1)$, By Lemma 1, we have

$$\begin{aligned}z(H_5-v_1) &= z(H_5-v_1-v_2)+\sum_{v'\in N_{H_5-v_1}(v_2)} z(H_5-v_1-\{v_2,v'\})\\ &= z(H_5-v_1-v_2)+z(H_5-v_1-\{v_2,v_3\})\\ &+(c-1)z(H_5-v_1-\{v_2,w\})\\ &= a(2d+1)+a(d+1)+(c-1)a(2d+1)\\ &= 2acd+ac+ad+a,\end{aligned}$$

where w is one pendent vertex adjacent to v_2 in H_5, $z(H_5-\{v_1,v_2\}) = a(2d+1)$, and $z(H_5-\{v_1,v_3\})=a(2c+1)$. Therefore,

$$\begin{aligned}z(H_5) &= (2acd+ac+ad+a)+a(2d+1)+a(2c+1)\\ &+(2cd+c+d+1)+(b-1)(2acd+ac+ad+a)\\ &= 2abcd+abc+abd+ab+2ac\\ &+2ad+2cd+2a+c+d+1 := g_5(a,b,c,d).\end{aligned}$$

Case 1. If $c-d\geq 2$, then

$$g_5(a,b,c-1,d+1)-g_5(a,b,c,d)=(2ab+2)(c-d-1)>0.$$

Case 2. If $d-c\geq 2$, this yields to

$$g_5(a,b,c+1,d-1)-g_5(a,b,c,d)=(2ab+2)(d-c-1)>0.$$

Cases 1 and 2 imply that, if H_5 has the maximum Hosoya index, we infer $|d-c|\leq 1$.

Case 3. If $a-b\geq 3$, then

$$\begin{aligned}g_5(a-1,b+1,c,d)-g_5(a,b,c,d) &= (2cd+c+d+1)(a-b-1)\\ &-2c-2d-2\\ &\geq 4cd>0.\end{aligned}$$

Case 4. If $b-a\geq 1$, then

$$\begin{aligned}g_5(a+1,b-1,c,d)-g_5(a,b,c,d) &= (2cd+c+d+1)(b-a-1)\\ &+2c+2d+2>0.\end{aligned}$$

Cases 3 and 4 imply that, if H_5 has the maximum Hosoya index, we conclude $0 \leq a-b \leq 2$.
Case 5. If $a-c \geq 2$, then

$$\begin{aligned} g_5(a-1,b,c+1,d) - g_5(a,b,c,d) &= (2bd+b+2)(a-c-1) \\ &\quad - bd - b - 1 \geq bd+1 > 0. \end{aligned}$$

Case 6. If $c-a \geq 1$, then

$$\begin{aligned} g_5(a+1,b,c-1,d) - g_5(a,b,c,d) &= (2bd+b+2)(c-a-1) \\ &\quad + bd + b + 1 > 0. \end{aligned}$$

Cases 5 and 6 imply that, if H_5 has the maximum Hosoya index, we conclude $0 \leq a-c \leq 1$.
From all above, we get the result. □

Let $\mathcal{V}_6$ be the set of unicyclic graphs of the form H_6 (as depicted in Figure 2), where v_1, v_2, v_3, v_4, and v_5 are five vertices with $a-1$, $b-1$, $c-1$, $d-1$, and $e-1$ pendent vertices, $a+b+c+d+e=n$, and $a,b,c,d,e \geq 1$. As the diameter is 4, from symmetry, we may assume a and c, or a and d, are at least 2. Let H_6^* be the graph of the form H_6 satisfying a,b,c,d,e almost equal.

Theorem 11. *The graph H_6^* has the maximum Hosoya index among all graphs in $\mathcal{V}_6$.*

Proof. For $H_6 \in \mathcal{V}_6$, by Lemmas 1 and 2, we have

$$\begin{aligned} z(H_6) &= z(H_6 - v_1) + \sum_{v' \in N_{H_6}(v_1)} z(H_6 - \{v_1, v'\}) \\ &= z(H_6 - v_1) + z(H_6 - \{v_1, v_2\}) + z(H_6 - \{v_1, v_5\}) \\ &\quad + (a-1) z(H_6 - \{v_1, y\}), \end{aligned}$$

where y is one pendent vertex adjacent to v_1 in H_6.
For $z(H_6 - v_1)$, by Lemma 1, we have

$$\begin{aligned} z(H_6 - v_1) &= z(H_6 - v_1 - v_2) + \sum_{v' \in N_{H_6 - v_1}(v_2)} z(H_6 - v_1 - \{v_2, v'\}) \\ &= z(H_6 - v_1 - v_2) + z(H_6 - v_1 - \{v_2, v_3\}) \\ &\quad + (b-1) z(H_6 - v_1 - \{v_2, v_{b-1}\}) \\ &= [z(H_6 - v_1 - v_2 - v_3) + z(H_6 - v_1 - v_2 - \{v_3, v_4\}) \\ &\quad + (c-1) z(H_6 - v_1 - v_2 - \{v_3, v_{c-1}\})] \\ &\quad + z(H_6 - v_1 - \{v_2, v_3\}) \\ &\quad + (b-1) z(H_6 - v_1 - \{v_2, v_{b-1}\}) \\ &= [(de+1) + e + (c-1)(de+1)] \\ &\quad + (de+1) + (b-1)(cde + c + e) \\ &= bcde + bc + be + de + 1, \end{aligned}$$

where v_{b-1} is one pendent vertex adjacent to v_2 in H_6, v_{c-1} is one pendent vertex adjacent to v_3,

$z(H_6 - \{v_1, v_2\}) = cde + c + e$, and

$$\begin{aligned} z(H_6 - \{v_1, v_5\}) &= z(H_6 - \{v_1, v_5\} - v_4) + z(H_6 - \{v_1, v_5\} \\ &\quad - \{v_4, v_3\}) + (d-1)z(H_6 - \{v_1, v_5\} \\ &\quad - \{v_4, v_{d-1}\}) \\ &= (bc+1) + b + (d-1)(bc+1) \\ &= bcd + b + d. \end{aligned}$$

Therefore, we obtain

$$\begin{aligned} z(H_6) &= (bcde + bc + be + de + 1) \\ &\quad + (cde + c + e) + (bcd + b + d) \\ &\quad + (a-1)(bcde + bc + be + de + 1) \\ &= abcde + abc + abe + ade \\ &\quad + bcd + cde + a + b + c + d + e. \end{aligned}$$

If $a - b \geq 2$, let H_6' be the graph obtained from H_6 by removing a pendent edge at v_1 to v_2. Then, we get

$$\begin{aligned} z(H_6') - z(H_6) &= (a-b-1)cde + (a-b-1)(c+e) - de + cd \\ &\geq cde + c + e - de + cd \\ &= (c-1)de + cd + c + e > 0. \end{aligned}$$

As a, b, c, d, e have the same status as depicted in Figure 2, we obtain that , when a, b, c, d, e are almost equal, H_6 has the maximal Hosoya index. □

Let $\mathcal{V}_7$ be the set of unicyclic graphs of the form H_7 (as depicted in Figure 2), where v_1, v_2, and v_3 are three vertices with $a-1$, $b-1$, and $c-1$ pendent vertices, $a + b + c = n - 3$, $a, b, c \geq 1$, and one of a, b, c is at least 2. Let H_7^* be the graph of the form H_7 satisfying a, b, c almost equal.

Theorem 12. *The graph H_7^* has the maximum Hosoya index among all graphs in $\mathcal{V}_7$.*

Proof. For $H_7 \in \mathcal{V}_7$, by Lemmas 1 and 2, we have

$$\begin{aligned} z(H_7) &= z(H_7 - v_1) + \sum_{v' \in N_{H_7}(v_1)} z(H_7 - \{v_1, v'\}) \\ &= z(H_7 - v_1) + z(H_7 - \{v_1, v_2\}) \\ &\quad + z(H_7 - \{v_1, v_6\}) + (a-1)z(H_7 - \{v_1, v_{a-1}\}), \end{aligned}$$

where v_{a-1} is one pendent vertex adjacent to v_1 in H_7.

For $z(H_7 - v_1)$, by Lemma 1, we have

$$\begin{aligned} z(H_7 - v_1) &= z(H_7 - v_1 - v_2) + \sum_{v' \in N_{H_7 - v_1}(v_2)} z(H_7 - v_1 - \{v_2, v'\}) \\ &= [3 + 2 + 3(c-1)] + 3 + (b-1)(3c+2) \\ &= 3bc + 2b + 3, \end{aligned}$$

where v_{c-1} is one pendent vertex adjacent to v_3, v_{b-1} is one pendent vertex adjacent to v_2 in H_7,

$z(H_7-\{v_1,v_2\})=3c+2$, and

$$\begin{aligned} z(H_7-\{v_1,v_6\}) &= [b(c+1)+1]+b(c+1) \\ &= 2bc+b+2. \end{aligned}$$

Therefore, we obtain

$$\begin{aligned} z(H_7) &= (3bc+2b+3)+(3c+2) \\ &+ (2bc+b+2)+(a-1)(3bc+2b+3) \\ &= 3abc+2ab+2bc+3a+b+3c+4 := g_7(a,b,c). \end{aligned}$$

Case 1. If $a-b\geq 2$, then

$$\begin{aligned} g_7(a-1,b+1,c)-g_7(a,b,c) &= (3c+2)(a-b-1) \\ &+ 2c-2 \geq 5c > 0. \end{aligned}$$

Case 2. If $b-a\geq 2$, then we conclude

$$\begin{aligned} g_7(a+1,b-1,c)-g_7(a,b,c) &= (3c+2)(b-a-1) \\ &- 2c+2 > 0. \end{aligned}$$

Cases 1 and 2 imply that, if H_7 has the maximum Hosoya index, we conclude $|a-b|\leq 1$. Similarly, by using symmetry, we may obtain $|c-b|\leq 1$.

Case 3. If $a-c\geq 2$, then

$$g_7(a-1,b,c+1)-g_7(a,b,c)=3b(a-c-1)>0.$$

Case 4. If $c-a\geq 2$, then get

$$g_7(a+1,b,c-1)-g_7(a,b,c)=3b(c-a-1)>0.$$

Cases 3 and 4 imply that, if H_7 has the maximum Hosoya index, we conclude $|a-c|\leq 1$.

In conclusion, when a,b,c are almost equal, H_7 has the maximal Hosoya index. □

Let $\mathcal{V}_8$ be the set of unicyclic graphs of the form H_8 (as depicted in Figure 2), where v_1, v_2, and v_3 are three vertices with $a-1$, $b-1$, and $c-1$ pendent vertices, $a+b+c=n-4$, $a,b,c\ \geq 1$, NS one of a,b,c is at least 2. Let H_8^* be the graph of the form H_8 satisfying a,b,c almost equal.

Theorem 13. *The graph H_8^* has the maximum Hosoya index among all graphs in $\mathcal{V}_8$.*

Proof. For $H_8\in\mathcal{V}_8$, by Lemmas 1 and 2, we have

$$\begin{aligned} z(H_8) &= z(H_8-v_1)+\sum_{v'\in N_{H_8}(v_1)} z(H_8-\{v_1,v'\}) \\ &= z(H_8-v_1)+z(H_8-\{v_1,v_2\}) \\ &+ z(H_8-\{v_1,v_7\})+(a-1)z(H_8-\{v_1,v_{1,a-1}\}), \end{aligned}$$

where v_{a-1} is one pendent vertex adjacent to v_1 in H_8.

For $z(H_8 - v_1)$, by Lemma 1, we have

$$\begin{aligned}
z(H_8 - v_1) &= z(H_8 - v_1 - v_2) \\
&+ \sum_{v' \in N_{H_8 - v_1}(v_2)} z(H_8 - v_1 - \{v_2, v'\}) \\
&= z(H_8 - v_1 - v_2) + z(H_8 - v_1 - \{v_2, v_3\}) \\
&+ (b-1) z(H_8 - v_1 - \{v_2, v_{b-1}\}) \\
&= [z(H_8 - v_1 - v_2 - v_3) \\
&+ z(H_8 - v_1 - v_2 - \{v_3, v_4\}) \\
&+ (c-1) z(H_8 - v_1 - v_2 - \{v_3, v_{c-1}\})] \\
&+ z(H_8 - v_1 - \{v_2, v_3\}) \\
&+ (b-1) z(H_8 - v_1 - \{v_2, v_{b-1}\}) \\
&= [5 + 3 + 5(c-1)] + 5 + (b-1)(5c+3) \\
&= 5bc + 3b + 5,
\end{aligned}$$

where v_{c-1} is one pendent vertex adjacent to v_3 in H_8, v_{b-1} is one pendent vertex adjacent to v_2 in H_8, $z(H_8 - \{v_1, v_2\}) = 5c + 3$, and

$$\begin{aligned}
z(H_8 - \{v_1, v_7\}) &= z(H_8 - \{v_1, v_7\} - v_6) \\
&+ z(H_8 - \{v_1, v_7\} - \{v_6, v_5\}) \\
&= z(H_8 - \{v_1, v_7\} - v_6 - v_5) \\
&+ z(H_8 - \{v_1, v_7\} - v_6 - \{v_5, v_4\})] \\
&+ z(H_8 - \{v_1, v_7\} - \{v_6, v_5\}) \\
&= 2[b(c+1) + 1] + bc + 1 \\
&= 3bc + 2b + 3.
\end{aligned}$$

Therefore,

$$\begin{aligned}
z(H_8) &= (5bc + 3b + 5) + (5c + 3) \\
&+ (3bc + 2b + 3) + (a-1)(5bc + 3b + 5) \\
&= 5abc + 3ab + 3bc + 5a + 2b + 5c + 6 := g_8(a, b, c).
\end{aligned}$$

Case 1. If $a - b \geq 2$, then

$$\begin{aligned}
g_8(a-1, b+1, c) - g_8(a, b, c) &= (5c+3)(a-b-1) \\
&+ 3c - 3 \geq 8c > 0.
\end{aligned}$$

Case 2. If $b - a \geq 2$, then

$$\begin{aligned}
g_8(a+1, b-1, c) - g_8(a, b, c) &= (5c+3)(b-a-1) \\
&- 3c + 3 \geq 2c + 6 > 0.
\end{aligned}$$

Cases 1 and 2 imply that, if H_8 has the maximum Hosoya index, we conclude $|a - b| \leq 1$. Similarly, we obtain $|c - b| \leq 1$.

Case 3. If $a - c \geq 2$, then

$$g_8(a-1, b, c+1) - g_8(a, b, c) = 5b(a-c-1) > 0.$$

Case 4. If $c - a \geq 2$, then we have

$$g_8(a+1, b, c-1) - g_8(a, b, c) = 5b(c - a - 1) > 0.$$

Cases 3 and 4 imply that, if H_8 has the maximum Hosoya index, we conclude $|a - c| \leq 1$.
In conclusion, when a, b, c are almost equal, H_8 has the maximal Hosoya index. □

Let $\mathcal{V}_9$ be the set of unicyclic graphs of the form H_9 (as depicted in Figure 2), where v_1, v_3, and v_5 are three vertices with $a-1$, $b-1$, and $c-1$ pendent vertices, $a+b+c = n-3$, $a, b, c \geq 1$, and one of a, b, c is at least 2. Let H_9^* be the graph of the form H_9 satisfying a, b, c almost equal.

Theorem 14. *The graph H_9^* has the maximum Hosoya index among all graphs in $\mathcal{V}_9$.*

Proof. For $H_9 \in \mathcal{V}_9$, from Lemmas 1 and 2, we have

$$\begin{aligned} z(H_9) &= z(H_9 - v_1) + \sum_{v' \in N_{H_9}(v_1)} z(H_9 - \{v_1, v'\}) \\ &= z(H_9 - v_1) + z(H_9 - \{v_1, v_2\}) \\ &+ z(H_9 - \{v_1, v_6\}) + (a-1)z(H_9 - \{v_1, v_{1,a-1}\}). \end{aligned}$$

For $z(H_9 - v_1)$, by Lemmas 1 and 2, we have

$$\begin{aligned} z(H_9 - v_1) &= z(H_9 - v_1 - v_2) \\ &+ \sum_{v' \in N_{H_9 - v_1}(v_2)} z(H_9 - v_1 - \{v_2, v'\}) \\ &= z(H_9 - v_1 - v_2) + z(H_9 - v_1 - \{v_2, v_3\}) \\ &= [z(H_9 - v_1 - v_2 - v_3) + z(H_9 - v_1 - v_2 - \{v_3, v_4\}) \\ &+ (b-1)z(H_9 - v_1 - v_2 - \{v_3, x\})] \\ &+ z(H_9 - v_1 - \{v_2, v_3\}) \\ &= [(c+2) + (c+1) + (b-1)(c+2)] + (c+2) \\ &= bc + 2b + 2c + 3. \end{aligned}$$

Here, x is a pendent vertex attached at v_3.
Observe that $z(H_9 - \{v_1, v_2\}) = bc + 2b + c + 1$,

$$\begin{aligned} z(H_9 - \{v_1, v_6\}) &= z(H_9 - \{v_1, v_6\} - v_5) \\ &+ z(H_9 - \{v_1, v_6\} - \{v_5, v_4\}) \\ &+ (c-1)z(H_9 - \{v_1, v_6\} - \{v_5, y\}) \\ &= (b+2) + (b+1) + (c-1)(b+2) \\ &= bc + b + 2c + 1, \end{aligned}$$

where y is one pendent vertex attached at v_5.
Thus, we obtain

$$\begin{aligned} z(H_9) &= z(H_9 - v_1) + z(H_9 - \{v_1, v_2\}) \\ &+ z(H_9 - \{v_1, v_6\}) + (a-1)z(H_9 - \{v_1, v_{1,a-1}\}) \\ &= (bc + 2b + 2c + 3) + (bc + 2b + c + 1) \\ &+ (bc + b + 2c + 1) + (a-1)(bc + 2b + 2c + 3) \\ &= abc + 2ab + 2ac + 2bc + 3a + 3b + 3c + 2 := g_9(a, b, c). \end{aligned}$$

If $a - b \geq 2$, then we have

$$\begin{aligned} & g_9(a-1, b+1, c) - g_9(a,b,c) \\ & = [(a-1)(b+1)c + 2(a-1)(b+1) \\ & + 2(a-1)c + 2(b+1)c + 3(a-1) \\ & + 3(b+1) + 3c + 2] \\ & - (abc + 2ab + 2ac + 2bc + 3a + 3b + 3c + 2) \\ & = (c+2)(a-b-1) \\ & \geq 0. \end{aligned}$$

Thus, we have $z(H_{91}) > z(H_9)$.

This implies that, if H_9 has the maximum Hosoya index, we conclude $|a-c| \leq 1$.

As b, c (resp. a, c) have the same status as shown in Figure 2, we also have $|b-c| \leq 1$. $|a-c| \leq 1$. This is the desired result. □

Theorem 15. *The graph H_6^* has the maximum Hosoya index among all graphs in $\mathcal{V}_n^4$ for $n \geq 50$.*

Proof. We need only compare $z(H_i^*)$ for $1 \leq i \leq 8$.

For H_1^*, as $0 \leq a-b \leq 1, 0 \leq a-c \leq 2, 0 \leq b-c \leq 1$, we have $b \leq a, c \leq a, c \leq b \leq a$, and $b \geq a-1, c \geq a-2$. Since $a+b+c = n-2$, we get $n-2 = a+b+c \geq a+a-1+a-2 = 3a-3$, this leads to $a \leq \frac{n+1}{3}$. Therefore,

$$\begin{aligned} z(H_1^*) &= 2abc + 2ab + 2a + 2c + 2 \\ &\leq 2a^3 + 2a^2 + 4a + 2 \\ &\leq \frac{2(n+1)^3}{27} + \frac{2(n+1)^2}{9} + \frac{4(n+1)}{3} + 2 := h_1(n) \end{aligned}$$

The last inequality holds for a function $f_1(a) = 2a^3 + 2a^2 + 4a + 2$ that is strictly increasing for $2 \leq a \leq \frac{n+1}{3}$.

For H_2^*, we have $0 \leq a-b \leq 2, 0 \leq a-c \leq 1, |c-d| \leq 1$. We may assume $0 \leq c-d \leq 1$ without loss of generality. Then, $b \leq a, c \leq a, d \leq c \leq a$, and $b \geq a-2, c \geq a-1, d \geq c-1 \geq a-2$. Thus, $n = a+b+c+d \geq a+a-2+a-1+a-2 = 4a-5$, and hence $a \leq \frac{n+5}{4}$. Therefore,

$$\begin{aligned} z(H_2^*) &= abcd + ab + ac + ad + cd + 1 \\ &\leq a^4 + 4a^2 + 1 \\ &\leq \frac{(n+5)^4}{256} + \frac{(n+5)^2}{4} + 1 := h_2(n). \end{aligned}$$

The last inequality holds for a function $f_2(a) = a^4 + 4a^2 + 1$ that is strictly increasing for $2 \leq a \leq \frac{n+5}{4}$.

For H_3^*, as a, b, c, d are almost equal and $a+b+c+d = n$, we have $a, b, c, d \leq \frac{n+3}{4}$

$$\begin{aligned} z(H_3^*) &= abcd + ab + ad + bc + cd + 2 \\ &\leq \frac{(n+3)^4}{256} + \frac{(n+3)^2}{4} + 2 := h_3(n). \end{aligned}$$

For H_4^*, $0 \le a-b \le 2, |c-d| \le 1, 0 \le a-c \le 1$. We may assume $0 \le c-d \le 1$ without loss of generality. Then, $b \le a, c \le a, d \le c \le a$, and $b \ge a-2, c \ge a-1, d \ge c-1 \ge a-2$. Thus, $n-1 = a+b+c+d \ge a+a-2+a-1+a-2 = 4a-5$, and hence $a \le \frac{n+4}{4}$. Therefore,

$$\begin{aligned} z(H_4^*) &= abcd + abc + abd + ac + ad + cd + 2a + c + d \\ &\le a^4 + 2a^3 + 3a^2 + 4a \\ &\le \left(\frac{n+4}{4}\right)^4 + 2\left(\frac{n+4}{4}\right)^3 + 3\left(\frac{n+4}{4}\right)^2 + 4\frac{n+4}{4} \\ &= \frac{(n+4)^4}{256} + \frac{(n+4)^3}{32} + \frac{3(n+4)^2}{16} + n + 4 := h_4(n). \end{aligned}$$

The last inequality holds for a function $f_3(a) = a^4 + 2a^3 + 3a^2 + 4a$ that is strictly increasing for $2 \le a \le \frac{n+4}{4}$.

For H_5^*, $0 \le a-b \le 2, |c-d| \le 1, 0 \le a-c \le 1$. We may assume $0 \le c-d \le 1$ without loss of generality. Then, $b \le a, c \le a, d \le c \le a$, and $b \ge a-2, c \ge a-1, d \ge c-1 \ge a-2$. Thus, $n-2 = a+b+c+d \ge a+a-2+a-1+a-2 = 4a-5$, and hence $a \le \frac{n+3}{4}$. Therefore,

$$\begin{aligned} z(H_5^*) &= 2abcd + abc + abd + ab \\ &\quad + 2ac + 2ad + 2cd + 2a + c + d + 1 \\ &\le 2a^4 + 2a^3 + 7a^2 + 4a + 1 \\ &\le 2\left(\frac{n+3}{4}\right)^4 + 2\left(\frac{n+3}{4}\right)^3 \\ &\quad + 7\left(\frac{n+3}{4}\right)^2 + 4\left(\frac{n+3}{4}\right) + 1 := h_5(n). \end{aligned}$$

The last inequality holds for a function $f_4(a) = 2a^4 + 2a^3 + 7a^2 + 4a + 1$ that is strictly increasing for $2 \le a \le \frac{n+3}{4}$.

For H_6^*, a, b, c, d, e are almost equal. Then, $a, b, c, d, e \ge \frac{n-4}{5}$ as $a+b+c+d+e = n$. Therefore,

$$\begin{aligned} z(H_6^*) &= abcde + abc + abe + ade + bcd + cde \\ &\quad + a + b + c + d + e \\ &\ge \left(\frac{n-4}{5}\right)^5 + 5\left(\frac{n-4}{5}\right)^3 + 5\frac{n-4}{5} := h_6(n). \end{aligned}$$

For H_7^*, a, b, c are almost equal. We may assume $a-1 \le b \le a+1, 0 \le a-c \le 1$. Then, we have $b \le a+1, c \le a$, and $b \ge a-1, c \ge a-1$. Thus, $n-3 = a+b+c \ge a+a-1+a-1 = 3a-2$, and hence $a \le \frac{n-1}{3}$. Therefore,

$$\begin{aligned} z(H_7^*) &= 3abc + 2ab + 2bc + 3a + b + 3c + 4 \\ &\le 3a^2(a+1) + 2a(a+1) + 2a(a+1) \\ &\quad + 3a + a + 1 + 3a + 4 \\ &= 3a^3 + 7a^2 + 11a + 5 \\ &\le 3\left(\frac{n-1}{3}\right)^3 + 7\left(\frac{n-1}{3}\right)^2 + 11\frac{n-1}{3} + 5 := h_7(n). \end{aligned}$$

The last inequality holds for a function $f_5(a) = 3a^3 + 7a^2 + 11a + 5$ which is strictly increasing for $1 \le a \le \frac{n-1}{3}$.

Let H_8^*, a,b,c are almost equal. We may assume $a-1 \le b \le a+1, 0 \le a-c \le 1$. Then, we have $b \le a+1, c \le a$, and $b \ge a-1, c \ge a-1$. Thus, $n-4 = a+b+c \ge a+a-1+a-1 = 3a-2$, and hence $a \le \frac{n-2}{3}$. Therefore,

$$\begin{aligned} z(H_8^*) &= 5abc + 3ab + 3bc + 5a + 2b + 5c + 6 \\ &\le 5a^2(a+1) + 3a(a+1) + 3a(a+1) \\ &+ 5a + 2(a+1) + 5a + 6 \\ &= 5a^3 + 11a^2 + 18a + 8 \\ &\le 5\left(\frac{n-2}{3}\right)^3 + 11\left(\frac{n-2}{3}\right)^2 + 18\frac{n-2}{3} + 8 := h_8(n). \end{aligned}$$

The last inequality holds for a function $f_6(a) = 5a^3 + 11a^2 + 18a + 8$ is strictly increasing for $1 \le a \le \frac{n-2}{3}$.

For H_9^*, since a,b,c are almost equal, We may assume $a-1 \le b \le a+1, 0 \le a-c \le 1$. Then $b \le a+1, c \le a$, $b \ge a-1, c \ge a-1$. As $n-3 = a+b+c \ge a+a-1+a-1 = 3a-2$, therefore $a \le \frac{n-1}{3}$. Thus, we have

$$\begin{aligned} z(H_9^*) =& abc + 2ab + 2ac + 2bc + 3a + 3b + 3c + 2 \\ &\le a^2(a+1) + 2a(a+1) + 2a^2 + 2a(a+1) \\ &+ 3a + 3(a+1) + 3a + 2 \\ &= a^3 + 7a^2 + 13a + 5 \\ &\le \left(\frac{n-1}{3}\right)^3 + 7\left(\frac{n-1}{3}\right)^2 + 13\frac{n-1}{3} + 5 := h_9(n). \end{aligned}$$

The last inequality holds as $f_7(a) = a^3 + 7a^2 + 13a + 5$ is strictly increasing for $1 \le a \le \frac{n-1}{3}$.

By using the software "Mathematica", we obtain the following comparison.

$h_2(n) - h_1(n) = \frac{1}{6912}(41{,}889 + 16{,}956n + 2706n^2 + 28n^3 + 27n^4) > 0$.

$h_2(n) - h_3(n) = \frac{1}{32}(164 + 81n + 12n^2 + n^3) > 0$.

$h_4(n) - h_2(n) = \frac{1}{256}(79 + 140n + 26n^2 + 4n^3) > 0$.

$h_6(n) - h_4(n) = \frac{1}{800{,}000}(-13{,}510{,}144 - 1{,}336{,}320n - 1{,}297{,}840n^2 - 2040n^3 - 8245n^4 + 256n^5) > 0$ for $n \ge 37$.

$h_8(n) - h_7(n) = \frac{1}{27}(-70 + 24n - 9n^2 + 2n^3) > 0$ for $n \ge 4$.

$h_7(n) - h_9(n) = \frac{1}{27}(16 - 12n - 6n^2 + 2n^3) \ge 0$ for $n \ge 4$.

$h_6(n) - h_8(n) = \frac{1}{84{,}375}(-531{,}148 - 315n - 67{,}155n^2 - 7390n^3 - 540n^4 + 27n^5) > 0$ for $n \ge 32$.

$h_6(n) - h_5(n) = \frac{1}{400{,}000}(-6{,}520{,}697 - 793{,}160n - 730{,}170n^2 - 13{,}520n^3 - 5685n^4 + 128n^5) > 0$ for $n \ge 50$.

The direct computation yields to $z(C_8) = 47, z(C_9) = 76$.

From the above discussion, we get the result. □

4. Summary and Conclusions

In this paper, we investigate extremal properties of the famous Hosoya index for unicyclic graphs with diameter at most four. There is no doubt that topological indices have been proven useful for analyzing molecules by means of their graph structure. Especially the Hosoya index is demanding to calculate for general graphs. Thus, special analytical results for the Hosoya index contribute to a better understanding of molecular topology when using this measure. Because of the problem of calculating the Hosoya index efficiently, we also believe that our results can be used for QSAR/QSPR problems. Moreover, the Hosoya index could be calculated on existing drugbanks to determine the value distributions and using them within QSAR/QSPR. Note that this index has a meaningful structural interpretation. As future work, we would like to continue to prove analytical results when establishing interrelations between the Hosoya index and known graph measures which have been proven useful for drug design and QSAR/QSPR.

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