Research Article

The Minimum Merrifield–Simmons Index of Unicyclic Graphs with Diameter at Most Four

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The Merrifield–Simmons index $i(G)$ of a graph G is defined as the number of subsets of the vertex set, in which any two vertices are nonadjacent, i.e., the number of independent vertex sets of G . In this paper, we determine the minimum Merrifield–Simmons index of unicyclic graphs with n vertices and diameter at most four.

1. Introduction

Numerous topological and chemical indices have been used for analyzing molecular graphs ([1–4]). The Merrifield–Simmons index was introduced by Merrifield and Simmons [5] in 1989. This index is one of the topological indices whose mathematical properties turned out to be applicable to several questions of molecular chemistry. For example, the connections with physico-chemical properties such as boiling point, entropy, or heat of vaporization are well studied.

Let $G = (V(G), E(G))$ denote a graph whose set of vertices and set of edges are $V(G)$ and $E(G)$, respectively. For any $v \in V(G)$, we denote the neighbors of v as $N_G(v)$, and $[v] = N_G(v) \cup \{v\}$. By n , we denote the number of vertices of G . All graphs considered here are both finite and simple. We denote, respectively, by S_n , P_n , and C_n the star, path, and cycle with n vertices. For other graph-theoretical terminology and notation, we refer to [6].

The Merrifield–Simmons index $i(G)$ of a graph G is defined as the number of subsets of the vertex set, in which any two vertices are nonadjacent, i.e., the number of independent vertex sets of G . Several papers deal with the Merrifield–Simmons index in several given graph classes. Usually, trees, unicyclic graphs, and certain structures involving pentagonal and hexagonal cycles are of major interest [7–15].

In this paper, we investigate the Merrifield–Simmons index $i(G)$ of unicyclic graphs with diameter at most four. We will give some results in Sections 3 and 4.

2. Some Notations and Lemmas

In this section, we gather notations which are used throughout this paper and give some necessary lemmas which will be used to prove our main results.

If $E' \subseteq E(G)$ and $W \subseteq V(G)$, then $G - E'$ and $G - W$ denote the subgraphs of G obtained by deleting the edges of E' and the vertices of W , respectively. By $f(n)$, we denote the n -th Fibonacci number, where $n \in \mathbb{N}$, $f(n) + f(n+1) = f(n+2)$, with initial conditions $f(0) = 0$ and $f(1) = 1$.

Lemma 1 (see [13]). Let $G = (V(G), E(G))$ be a graph.

- (i) If $G_1, G_2, \dots, G_m$ are the components of the graph G , then $i(G) = \prod_{i=1}^m i(G_i)$;
- (ii) If $x \in V(G)$, then $i(G) = i(G - \{x\}) + i(G - [x])$.

Lemma 2 (see [8]). Let $G = (V(G), E(G))$ be a graph. Then, $i(S_n) = 2^{n-1} + 1$; $i(P_n) = f(n+2)$, for any $n \in \mathbb{N}$; $i(C_n) = f(n-1) + f(n+1)$, for any $n \geq 3$.

3. The Unicyclic Graphs with Diameter Three

In this section, we study the minimal Merrifield–Simmons index of unicyclic graphs with n vertices and diameter three.

Let $\mathcal{U}_n^3$ be the set of all unicyclic graphs with n vertices and diameter three. 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 three cycles C_5 , C_6 , and C_7 are all members of the unicyclic graphs with diameter three.

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 , and $c \geq 1$, and at least two of a, b , and c are greater than 2. Let graph G_1^* be the graph of the form G_1 , satisfying a, b, c almost equal, that is, $|a - b| \leq 1$, $|b - c| \leq 1$, and $|c - a| \leq 1$.

Theorem 1. *The graph G_1^* has the minimum Merrifield–Simmons 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 get

$$\begin{aligned} i(G_1) &= i(G_1 - \{v_1\}) + i(G_1 - [v_1]) \\ &= [i(P_1)]^{a-1} [i(P_1)]^{b-1} \cdot i(S_c) + [i(P_1)]^{c-1} \\ &\quad + [i(P_1)]^{b+c-2} \\ &= 2^{a-1} [2^{b-1} \cdot (2^{c-1} + 1) + 2^{c-1}] + 2^{b+c-2} \\ &= 2^{n-3} + 2^{a+b-2} + 2^{a+c-2} + 2^{b+c-2} := f_1(a, b, c). \end{aligned} \quad (1)$$

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

$$f_1(a + 1, b - 1, c) - f_1(a, b, c) = 2^{b+c-3} (2^{a+1-b} - 1) < 0. \quad (2)$$

Obviously, a, b, c have the same status in $f_1(a, b, c)$; we infer $|a - b| \leq 1$; further, $|b - c| \leq 1$ and $|c - a| \leq 1$. Thus, when a, b , and c are almost equal, graph G_1 has the minimal Merrifield–Simmons index.

Let $\mathcal{U}_2$ be the set of unicyclic graphs of the form G_2 (as depicted in Figure 2), where $a + b = n - 2$, $a \geq 2$, and $b \geq 1$. Let graph 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 minimum Merrifield–Simmons index among all graphs in $\mathcal{U}_2$.*

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

$$\begin{aligned} i(G_2) &= i(G_2 - \{v_1\}) + i(G_2 - [v_1]) \\ &= [i(P_2)] [i(P_1)]^{b-1} [i(S_a)] + [i(P_1)]^{a-1} \\ &= 3 [2^{b-1} \cdot (2^{a-1} + 1)] + 2^{a-1} \\ &= 3 \cdot 2^{n-4} + 3 \cdot 2^{b-1} + 2^{a-1} := f_2(a, b). \end{aligned} \quad (3)$$

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

FIGURE 1: Unicyclic graphs with diameter three G_1 .

FIGURE 2: Unicyclic graphs with diameter three G_2 .

$$f_2(a + 1, b - 1) - f_2(a, b) = 2^{a-1} (1 - 3 \cdot 2^{b-a-1}) < 0. \quad (4)$$

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

$$f_2(a - 1, b + 1) - f_2(a, b) = 2^{a-2} (3 \cdot 2^{b-a+1} - 1) < 0. \quad (5)$$

Therefore, graph G_2^* , where $0 \leq a - b \leq 2$, is the minimum Merrifield–Simmons index among all graphs in $\mathcal{U}_2$.

Let $\mathcal{U}_3$ be the set of unicyclic graphs of the form G_3 (as depicted in Figure 3), 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 graph G_3^* be the graph of the form G_3 , satisfying a, b almost equal, that is, $|a - b| \leq 1$.

Theorem 3. *The graph G_3^* has the minimum Merrifield–Simmons index among all graphs in $\mathcal{U}_3$.*

Proof. Assume $G_3 \in \mathcal{U}_3$ with $a \geq b \geq 1$. By Lemmas 1 and 2, we get

$$\begin{aligned} i(G_3) &= i(G_3 - \{v_1\}) + i(G_3 - [v_1]) \\ &= [i(P_1)]^{a-1} [i(P_2) [i(P_1)]^{b-1} + i(P_1)] \\ &\quad + [i(P_1)]^{b-1} i(P_1) \\ &= 2^{a-1} [3 \cdot 2^{b-1} + 2] + 2^b \\ &= 3 \cdot 2^{n-4} + 2^b + 2^a := f_3(a, b). \end{aligned} \quad (6)$$

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

$$f_3(a - 1, b + 1) - f_3(a, b) = 2^b (1 - 2^{a-b-1}) < 0. \quad (7)$$

FIGURE 3: Unicyclic graphs with diameter three G_3 .

Obviously, a, b have the same status in $f_3(a, b)$; we infer $|a - b| \leq 1$. Thus, when a, b are almost equal, graph G_3 has the minimal Merrifield-Simmons index.

Let $\mathcal{U}_4$ be the set of unicyclic graphs of the form G_4 (as depicted in Figure 4), where v_1 and v_2 are two vertices with $a - 1, b - 1$ pendent vertices, satisfying $a + b = n - 3, a, b \geq 1$. Let graph G_4^* be the graph of the form G_4 , satisfying a, b almost equal, that is, $|a - b| \leq 1$.

Theorem 4. *The graph G_4^* has the minimum Merrifield-Simmons index among all graphs in $\mathcal{U}_4$.*

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

$$\begin{aligned}
 i(G_4) &= i(G_4 - \{v_1\}) + i(G_4 - [v_1]) \\
 &= [i(P_1)]^{a-1} [i(P_1)]^{b-1} [i(P_3)] + i(P_2) \\
 &\quad + i(P_2)[i(P_1)]^{b-1} \\
 &= 2^{a-1} [5 \cdot 2^{b-1} + 3] + 3 \cdot 2^{b-1} \\
 &= 5 \cdot 2^{n-5} + 3 \cdot 2^{b-1} + 3 \cdot 2^{a-1} := f_4(a, b).
 \end{aligned} \tag{8}$$

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

$$f_4(a - 1, b + 1) - f_4(a, b) = 3 \cdot 2^{b-1} (1 - 2^{a-b-1}) < 0. \tag{9}$$

Obviously, a, b have the same status in $f_4(a, b)$; we infer $|a - b| \leq 1$. Thus, when a, b are almost equal, graph G_4 has the minimal Merrifield-Simmons index.

Theorem 5. *The graph G_1^* has the minimum Merrifield-Simmons index among all graphs in $\mathcal{U}_n^3$ if $n \geq 8$.*

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

For G_1^* , we assume that $a \leq b \leq c$. Since a, b, c are almost equal and $a + b + c = n$, then $a \geq (n - 2/3)$. We have

$$\begin{aligned}
 i(G_1^*) &= 2^{n-3} + 2^{a+b-2} + 2^{a+c-2} + 2^{b+c-2} \\
 &\geq 2^{n-3} + 3 \cdot 2^{2a-2} \\
 &\geq 2^{n-3} + 3 \cdot 2^{(2n-10)/3} := g_1(n).
 \end{aligned} \tag{10}$$

FIGURE 4: Unicyclic graphs with diameter three G_4 .

For G_2^* , as $0 \leq a - b \leq 2$ and $a + b = n - 2$, we have $a - 2 \leq b \leq a$ and $a \geq (n - 2/2)$. Thus,

$$\begin{aligned}
 i(G_2^*) &= 3 \cdot 2^{n-4} + 3 \cdot 2^{b-1} + 2^{a-1} \\
 &\geq 3 \cdot 2^{n-4} + 3 \cdot 2^{a-2-1} + 2^{a-1} \\
 &\geq 3 \cdot 2^{n-4} + 7 \cdot 2^{(n-8)/2} := g_2(n).
 \end{aligned} \tag{11}$$

For G_3^* , as $|a - b| \leq 1$ and $a + b = n - 2$, we have $a - 1 \leq b \leq a + 1$ and $a \geq (n - 3/2)$. Thus,

$$\begin{aligned}
 i(G_3^*) &= 3 \cdot 2^{n-4} + 2^b + 2^a \\
 &\geq 3 \cdot 2^{n-4} + 2^{a-1} + 2^a \\
 &\geq 3 \cdot 2^{n-4} + 3 \cdot 2^{(n-5)/2} := g_3(n).
 \end{aligned} \tag{12}$$

For G_4^* , as $|a - b| \leq 1$ and $a + b = n - 3$, we have $a - 1 \leq b \leq a + 1$ and $a \geq (n - 4/2)$. Thus,

$$\begin{aligned}
 i(G_4^*) &= 5 \cdot 2^{n-5} + 3 \cdot 2^{b-1} + 3 \cdot 2^{a-1} \\
 &\geq 5 \cdot 2^{n-5} + 3 \cdot 2^{a-1-1} + 3 \cdot 2^{a-1} \\
 &\geq 5 \cdot 2^{n-5} + 9 \cdot 2^{(n-8)/2} := g_4(n).
 \end{aligned} \tag{13}$$

By simple calculation comparison, we obtain the following comparison: $g_3(n) - g_2(n) = 2^{(n-8/2)} (6\sqrt{2} - 7) > 0$, for $n \geq 8$. $g_2(n) - g_4(n) = 2^{(n-4/2)} (2^{(n-6/2)} - 1) > 0$, for $n \geq 8$. $g_4(n) - g_1(n) = 2^{(n-8/2)} (2^{(n-2/2)} + 9 - 3 \cdot 2^{(n-4/6)}) > 0$, for $n \geq 2$. Thus, $g_1(n) \leq g_4(n) \leq g_2(n) \leq g_3(n)$, for $n \geq 8$. A direct computation yields $i(C_5) = 11$, $i(C_6) = 18$, and $i(C_7) = 29$. Thus, the graph G_1^* has the minimum Merrifield-Simmons index among all graphs in $\mathcal{U}_n^3$ if $n \geq 8$. From above, we obtain the result.

4. The Unicyclic Graphs with Diameter Four

In this section, we study the minimal Merrifield-Simmons index of unicyclic graphs with n vertices and diameter four.

Let $\mathcal{V}_n^4$ be the set of all unicyclic graphs with n vertices and diameter four. 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 graph of the form H_i , $i = 1, 2, 3, 4, 5, 6, 7, 8, 9$. 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 four.

Let $\mathcal{V}_1$ be the set of unicyclic graphs of the form H_1 (as depicted in Figure 5), where v_1, v_4 , and v_5 are three vertices with $c-1$, $b-1$, and $a-1$ pendent vertices, $a+b+c=n-2$, $a \geq 2$, $b \geq 1$, and $c \geq 1$. Let graph H_1^* be the graph of the form H_1 , satisfying $0 \leq a-b \leq 1$, $0 \leq a-c \leq 2$, and $0 \leq b-c \leq 2$.

Theorem 6. *The graph H_1^* has the minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_1$.*

Proof. Assume $H_1 \in \mathcal{V}_1$. By Lemmas 1 and 2, we get

$$\begin{aligned}
 i(H_1) &= i(H_1 - \{v_1\}) + i(H_1 - [v_1]) \\
 &= i(P_2)i(P_1)^{c-1} [i(P_1)^{b-1}i(S_a) + i(P_1)^{a-1}] \\
 &\quad + i(P_1)^{b-1}i(S_a) \\
 &= 3 \cdot 2^{c-1} [2^{b-1}(2^{a-1} + 1) + 2^{a-1}] + 2^{b-1}(2^{a-1} + 1) \\
 &= 3 \cdot 2^{n-5} + 3 \cdot 2^{a+c-2} + 3 \cdot 2^{b+c-2} + 2^{b+a-2} + 2^{b-1} \\
 &:= f_1(a, b, c).
 \end{aligned} \tag{14}$$

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

$$\begin{aligned}
 f_1(a+1, b-1, c) - f_1(a, b, c) \\
 &= 3 \cdot 2^{a+c-2} - 3 \cdot 2^{b+c-3} - 2^{b-2} \\
 &\leq 3 \cdot 2^{b-1+c-2} - 3 \cdot 2^{b+c-3} - 2^{b-2} \\
 &= -2^{b-2} < 0.
 \end{aligned} \tag{15}$$

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

$$\begin{aligned}
 f_1(a-1, b+1, c) - f_1(a, b, c) \\
 &= -3 \cdot 2^{a+c-3} + 3 \cdot 2^{b+c-2} + 2^{b-1} \\
 &\leq -3 \cdot 2^{b+2+c-3} + 3 \cdot 2^{b+c-2} + 2^{b-1} \\
 &= 2^{b-1}(1 - 3 \cdot 2^{c-1}) < 0.
 \end{aligned} \tag{16}$$

These imply that, if H_1 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_1$, then we infer $0 \leq a-b \leq 1$.

If $c-a \geq 1$, then we have

$$\begin{aligned}
 f_1(a+1, b, c-1) - f_1(a, b, c) \\
 &= -3 \cdot 2^{b+c-3} + 2^{b+a-2} \\
 &\leq -3 \cdot 2^{b+a+1-3} + 2^{b+a-2} \\
 &= -2^{a+b-1} < 0.
 \end{aligned} \tag{17}$$

If $a-c \geq 3$, then we have

$$\begin{aligned}
 f_1(a-1, b, c+1) - f_1(a, b, c) \\
 &= 3 \cdot 2^{b+c-2} - 2^{b+a-3} \\
 &\leq 3 \cdot 2^{b+c-2} - 2^{b+c+3-3} \\
 &= -2^{c+b-2} < 0.
 \end{aligned} \tag{18}$$

FIGURE 5: Unicyclic graphs with diameter three H_1 .

These imply that, if H_1 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_1$, then we infer $0 \leq a-c \leq 2$.

If $c-b \geq 1$, then we have

$$\begin{aligned}
 f_1(a, b+1, c-1) - f_1(a, b, c) \\
 &= -3 \cdot 2^{a+c-3} + 2^{a+b-2} + 2^{b-1} \\
 &\leq -3 \cdot 2^{a+b-2} + 2^{a+b-2} + 2^{b-1} \\
 &= 2^{b-1}(1 - 2^a) < 0.
 \end{aligned} \tag{19}$$

If $b-c \geq 3$, then we have

$$\begin{aligned}
 f_1(a, b-1, c+1) - f_1(a, b, c) \\
 &= 3 \cdot 2^{a+c-2} - 2^{a+b-3} - 2^{b-2} \\
 &\leq 3 \cdot 2^{a+b-5} - 2^{a+b-3} - 2^{b-2} \\
 &= -2^{b-2} - 2^{a+b-5} < 0.
 \end{aligned} \tag{20}$$

These imply that, if H_1 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_1$, then we infer $0 \leq b-c \leq 2$.

Let $\mathcal{V}_2$ be the set of unicyclic graphs of the form H_2 (as depicted in Figure 6), where v_1, v_2, v_3 , and v_4 are four vertices with $b-1$, $c-1$, $d-1$, and $a-1$ pendent vertices, $a+b+c+d=n$. As the diameter is 4, we infer $a \geq 2$ and $b \geq 1$, and one value of c and d is at least 2. Let graph H_2^* be the graph of the form H_2 , satisfying $0 \leq a-b \leq 2$, $0 \leq c-b \leq 1$, $0 \leq c-d \leq 1$, $0 \leq a-d \leq 2$, $0 \leq a-c \leq 1$, and $0 \leq d-b \leq 1$.

Theorem 7. *The graph H_2^* has the minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_2$.*

Proof. Assume $H_2 \in \mathcal{V}_2$. By Lemmas 1 and 2, we get

$$\begin{aligned}
 i(H_2) &= i(H_2 - \{v_1\}) + i(H_2 - [v_1]) \\
 &= i(P_1)^{b-1}i(S_a) [i(P_1)^{d-1}i(S_c) + i(P_1)^{c-1}] \\
 &\quad + i(P_1)^{a+c+d-3} \\
 &= 2^{b-1}(2^{a-1} + 1) [2^{d-1}(2^{c-1} + 1) + 2^{c-1}] + 2^{a+c+d-3} \\
 &= 2^{n-4} + 2^{a+c+d-3} + 2^{a+b+d-3} + 2^{b+c+d-3} + 2^{a+b+c-3} \\
 &\quad + 2^{b+d-2} + 2^{b+c-2} := f_2(a, b, c, d).
 \end{aligned} \tag{21}$$

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

FIGURE 6: Unicyclic graphs with diameter three H_2 .

$$\begin{aligned}
 & f_2(a+1, b-1, c, d) - f_2(a, b, c, d) \\
 &= 2^{a+c+d-3} - 2^{b+c+d-4} - 2^{b+d-3} - 2^{b+c-3} \\
 &\leq 2^{b-1+c+d-3} - 2^{b+c+d-4} - 2^{b+d-3} - 2^{b+c-3} \\
 &= -2^{b+d-3} - 2^{b+c-3} < 0.
 \end{aligned} \tag{22}$$

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

$$\begin{aligned}
 & f_2(a-1, b+1, c, d) - f_2(a, b, c, d) \\
 &= -2^{a+c+d-4} + 2^{b+c+d-3} + 2^{b+d-2} + 2^{b+c-2} \\
 &\leq -2^{b+3+c+d-4} + 2^{b+c+d-3} + 2^{b+d-2} + 2^{b+c-2} \\
 &= 2^{b+c+d-3} (2^{1-c} + 2^{1-d} - 3) < 0.
 \end{aligned} \tag{23}$$

These imply that, if H_2 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_2$, then we infer $0 \leq a-b \leq 2$.

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

$$\begin{aligned}
 & f_2(a, b+1, c-1, d) - f_2(a, b, c, d) \\
 &= -2^{a+c+d-4} + 2^{b+a+d-3} + 2^{b+d-2} \\
 &\leq -2^{a+b+2+d-4} + 2^{b+a+d-3} + 2^{b+d-2} \\
 &= 2^{b+d-2} (1 - 2^{a-1}) < 0.
 \end{aligned} \tag{24}$$

If $b-c \geq 1$, then we have

$$\begin{aligned}
 & f_2(a, b-1, c+1, d) - f_2(a, b, c, d) \\
 &= 2^{a+c+d-3} - 2^{b+a+d-4} - 2^{b+d-3} \\
 &\leq 2^{a+b-1+d-3} - 2^{b+a+d-4} - 2^{b+d-3} \\
 &= -2^{b+d-3} < 0.
 \end{aligned} \tag{25}$$

These imply that, if H_2 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_2$, then we infer $0 \leq c-b \leq 1$.

If $c-d \geq 2$, then we have

$$\begin{aligned}
 & f_2(a, b, c-1, d+1) - f_2(a, b, c, d) \\
 &= -2^{a+b+c-4} + 2^{b+a+d-3} + 2^{b+d-2} - 2^{b+c-3} \\
 &\leq -2^{a+b+d+2-4} + 2^{b+a+d-3} + 2^{b+d-2} - 2^{b+d+2-3} \\
 &= -2^{a+b+d-3} - 2^{b+d-2} < 0.
 \end{aligned} \tag{26}$$

If $d-c \geq 1$, then we have

$$\begin{aligned}
 & f_2(a, b, c+1, d-1) - f_2(a, b, c, d) \\
 &= 2^{a+b+c-3} - 2^{b+a+d-4} - 2^{b+d-3} + 2^{b+c-2} \\
 &\leq 2^{a+b+d-1-3} - 2^{b+a+d-4} - 2^{b+d-3} + 2^{b+d-1-3} \\
 &= -2^{b+d-4} < 0.
 \end{aligned} \tag{27}$$

These imply that, if H_2 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_2$, then we infer $0 \leq c-d \leq 1$.

If $d-a \geq 1$, then we have

$$\begin{aligned}
 & f_2(a+1, b, c, d-1) - f_2(a, b, c, d) \\
 &= -2^{b+c+d-4} + 2^{a+b+c-3} - 2^{b+d-3} \\
 &\leq -2^{b+c+a+1-4} + 2^{a+b+c-3} - 2^{b+a+1-3} \\
 &= -2^{b+a-2} < 0.
 \end{aligned} \tag{28}$$

If $a-d \geq 3$, then we have

$$\begin{aligned}
 & f_2(a-1, b, c, d+1) - f_2(a, b, c, d) \\
 &= 2^{b+c+d-3} - 2^{a+b+c-4} + 2^{b+d-2} \\
 &\leq 2^{b+c+a-3-3} - 2^{a+b+c-4} + 2^{b+a-3-2} \\
 &= 2^{b+a-5} (1 - 3 \cdot 2^{c-1}) < 0.
 \end{aligned} \tag{29}$$

These imply that, if H_2 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_2$, then we infer $0 \leq a-d \leq 2$.

If $c-a \geq 1$, then we have

$$\begin{aligned}
 & f_2(a+1, b, c-1, d) - f_2(a, b, c, d) \\
 &= 2^{a+b+d-3} - 2^{b+c+d-4} - 2^{b+c-3} \\
 &\leq 2^{c-1+b+d-3} - 2^{b+c+d-4} - 2^{b+c-3} \\
 &= -2^{b+c-3} < 0.
 \end{aligned} \tag{30}$$

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

$$\begin{aligned}
 & f_2(a-1, b, c+1, d) - f_2(a, b, c, d) \\
 &= -2^{a+b+d-4} + 2^{b+c+d-3} + 2^{b+c-2} \\
 &\leq -2^{c+2+b+d-4} + 2^{b+c+d-3} + 2^{b+c-2} \\
 &= 2^{b+c-2} (1 - 2^{d-1}) < 0.
 \end{aligned} \tag{31}$$

These imply that, if H_2 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_2$, then we infer $0 \leq a-c \leq 1$.

If $b-d \geq 1$, then we have

$$\begin{aligned}
 & f_2(a, b-1, c, d+1) - f_2(a, b, c, d) \\
 &= 2^{a+c+d-3} - 2^{a+b+c-4} - 2^{b+c-3} \\
 &\leq 2^{a+c+b-1-3} - 2^{a+b+c-4} - 2^{b+c-3} \\
 &= -2^{b+c-3} < 0.
 \end{aligned} \tag{32}$$

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

$$\begin{aligned}
& f_2(a, b+1, c, d-1) - f_2(a, b, c, d) \\
&= -2^{a+c+d-4} + 2^{a+b+c-3} + 2^{b+c-2} \\
&\leq -2^{a+c+b+2-4} + 2^{a+b+c-3} + 2^{b+c-2} \\
&= 2^{b+c-2}(1 - 2^{a-1}) < 0.
\end{aligned} \tag{33}$$

These imply that, if H_2 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_2$, then we infer $0 \leq d - b \leq 1$.

Let $\mathcal{V}_3$ be the set of unicyclic graphs of the form H_3 (as depicted in Figure 7), 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 , and $d \geq 1$. As the diameter is 4, a and c , or b and d , are at least 2. Let graph H_3^* be the graph of the form H_3 , satisfying a, b, c , and d almost equal, that is, $\forall x, y \in \{a, b, c, d\}$, $x \neq y$, and $|x - y| \leq 1$.

Theorem 8. *The graph H_3^* has the minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_3$.*

Proof. Assume $H_3 \in \mathcal{V}_3$. By Lemmas 1 and 2, we get

$$\begin{aligned}
i(H_3) &= i(H_3 - \{v_1\}) + i(H_3 - [v_1]) \\
&= i(P_1)^{a-1} [i(S_b)i(S_d)i(P_1)^{c-1} + i(P_1)^{b+d-2}] \\
&\quad + i(P_1)^{b+d-2}i(S_c) \\
&= 2^{a-1} [2^{c-1}(2^{b-1}+1)(2^{d-1}+1) + 2^{b+d-2}] \\
&\quad + 2^{b+d-2}(2^{c-1}+1) \\
&= 2^{n-4} + 2^{a+c+d-3} + 2^{a+b+d-3} + 2^{b+c+d-3} \\
&\quad + 2^{a+b+c-3} + 2^{b+d-2} + 2^{a+c-2} := f_3(a, b, c, d).
\end{aligned} \tag{34}$$

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

$$\begin{aligned}
& f_3(a-1, b+1, c, d) - f_3(a, b, c, d) \\
&= -2^{a+c+d-4} + 2^{b+c+d-3} - 2^{a+c-3} + 2^{b+d-2} \\
&\leq -2^{b+2+c+d-4} + 2^{b+c+d-3} - 2^{b+2+c-3} + 2^{b+d-2} \\
&= -2^{b+d-2}(2^{c-1}-1) - 2^{b+c-1} < 0.
\end{aligned} \tag{35}$$

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

$$\begin{aligned}
& f_3(a+1, b-1, c, d) - f_3(a, b, c, d) \\
&= 2^{a+c+d-3} - 2^{b+c+d-4} + 2^{a+c-2} - 2^{b+d-3} \\
&\leq 2^{a+c+d-3} - 2^{a+2+c+d-4} + 2^{a+c-2} - 2^{a+2+d-3} \\
&= -2^{a+c-2}(2^{d-1}-1) - 2^{a+d-1} < 0.
\end{aligned} \tag{36}$$

These imply that, if H_3 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_3$, then we infer $|a - b| \leq 1$. Obviously, as $f_3(a, b, c, d) = f_3(c, b, a, c)$, we can get $|c - b| \leq 1$. Similarly, we have $|c - d| \leq 1$ and $|a - d| \leq 1$ by $f_3(a, b, c, d) = f_3(a, d, c, b)$.

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

FIGURE 7: Unicyclic graphs with diameter three H_3 .

$$\begin{aligned}
& f_3(a-1, b, c+1, d) - f_3(a, b, c, d) \\
&= 2^{a+b+d-4} + 2^{b+c+d-2} - 2^{a+b+d-3} - 2^{b+c+d-3} \\
&= 2^{b+c+d-3} - 2^{a+b+d-4} \\
&= 2^{b+c+d-3}(1 - 2^{a-c-1}) < 0.
\end{aligned} \tag{37}$$

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

$$\begin{aligned}
& f_3(a+1, b, c-1, d) - f_3(a, b, c, d) \\
&= 2^{a+b+d-2} + 2^{b+c+d-4} - 2^{a+b+d-3} - 2^{b+c+d-3} \\
&= 2^{a+b+d-3} - 2^{b+c+d-4} \\
&= 2^{a+b+d-3}(1 - 2^{c-a-1}) < 0.
\end{aligned} \tag{38}$$

These imply that, if H_3 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_3$, then we infer $|a - c| \leq 1$.

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

$$\begin{aligned}
& f_3(a, b-1, c, d+1) - f_3(a, b, c, d) \\
&= 2^{a+b+c-4} + 2^{a+c+d-2} - 2^{a+b+c-3} - 2^{a+c+d-3} \\
&= 2^{a+c+d-3} - 2^{a+b+c-4} \\
&= 2^{a+c+d-3}(1 - 2^{b-d-1}) < 0.
\end{aligned} \tag{39}$$

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

$$\begin{aligned}
& f_3(a, b+1, c, d-1) - f_3(a, b, c, d) \\
&= 2^{a+b+c-2} + 2^{a+c+d-4} - 2^{a+b+c-3} - 2^{a+c+d-3} \\
&= 2^{a+b+c-3} - 2^{a+c+d-4} \\
&= 2^{a+b+c-3}(1 - 2^{d-b-1}) < 0.
\end{aligned} \tag{40}$$

These imply that, if H_3 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_3$, then we infer $|b - d| \leq 1$.

Let $\mathcal{V}_4$ be the set of unicyclic graphs of the form H_4 (as depicted in Figure 8), where v_1, v_2, v_4 , and v_5 are four vertices with $b-1$, $c-1$, $d-1$, and $a-1$ pendent vertices, $a+b+c+d=n-1$, $a \geq 2$, b, c , and $d \geq 1$. Let graph H_4^* be the graph of the form H_4 , satisfying $0 \leq a - b \leq 2$, $0 \leq c - b \leq 1$, $|c - d| \leq 1$, $0 \leq a - d \leq 1$, $0 \leq a - c \leq 1$, and $|d - b| \leq 1$.

FIGURE 8: Unicyclic graphs with diameter three H_4 .

Theorem 9. The graph H_4^* has the minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_4$.

Proof. Assume $H_4 \in \mathcal{V}_4$. By Lemmas 1 and 2, we get

$$\begin{aligned}
 i(H_4) &= i(H_4 - \{v_1\}) + i(H_4 - [v_1]) \\
 &= i(P_1)^{b-1} i(S_a) [i(S_c) i(S_d) + i(P_1)^{c+d-2}] \\
 &\quad + i(P_1)^{a+c+d-2} \\
 &= 2^{b-1} (2^{a-1} + 1) [(2^{c-1} + 1)(2^{d-1} + 1) + 2^{c+d-2}] \\
 &\quad + 2^{a+c+d-2} \\
 &= 2^{n-4} + 2^{a+b+d-3} + 2^{a+b+c-3} + 2^{b+c+d-2} + 2^{a+c+d-2} \\
 &\quad + 2^{a+b-2} + 2^{b+c-2} + 2^{b+d-2} + 2^{b-1} := f_4(a, b, c, d).
 \end{aligned} \tag{41}$$

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

$$\begin{aligned}
 f_4(a-1, b+1, c, d) - f_4(a, b, c, d) &= -2^{a+c+d-3} + 2^{b+c+d-2} + 2^{b+d-2} + 2^{b+c-2} + 2^{b-1} \\
 &\leq -3 \cdot 2^{b+c+d-2} + 2^{b+d-2} + 2^{b+c-2} + 2^{b-1} \\
 &= 2^{b-1} [(1 - 2^{c+d-1}) + 2^{d-1}(1 - 2^c) + 2^{c-1}(1 - 2^d)] < 0.
 \end{aligned} \tag{42}$$

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

$$\begin{aligned}
 f_4(a+1, b-1, c, d) - f_4(a, b, c, d) &= 2^{a+c+d-2} - 2^{b+c+d-3} - 2^{b+d-3} - 2^{b+c-3} - 2^{b-2} \\
 &\leq 2^{b-1+c+d-2} - 2^{b+c+d-3} - 2^{b+d-3} - 2^{b+c-3} - 2^{b-2} \\
 &= -2^{b+d-3} - 2^{b+c-3} - 2^{b-2} < 0.
 \end{aligned} \tag{43}$$

These imply that, if H_4 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_4$, then we infer $0 \leq a - b \leq 2$.

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

$$\begin{aligned}
 f_4(a, b+1, c-1, d) - f_4(a, b, c, d) &= 2^{a+b+d-3} - 2^{a+c+d-3} + 2^{b+a-2} + 2^{b+d-2} + 2^{b-1} \\
 &\leq 2^{a+b+d-3} - 2^{a+b+2+d-3} + 2^{b+a-2} + 2^{b+d-2} + 2^{b-1} \\
 &= 2^{b-1} [(1 - 2^{a+d-1}) + 2^{a-1}(1 - 2^{d-1}) + 2^{d-1}(1 - 2^{a-1})] \\
 &< 0.
 \end{aligned} \tag{44}$$

If $b - c \geq 1$, then we have

$$\begin{aligned}
 f_4(a, b-1, c+1, d) - f_4(a, b, c, d) &= -2^{a+b+d-4} + 2^{a+c+d-3} - 2^{b+d-3} - 2^{b+a-3} - 2^{b-2} \\
 &\leq -2^{a+b+d-4} + 2^{a+b-1+d-3} - 2^{b+d-3} - 2^{b+a-3} - 2^{b-2} \\
 &= -2^{b+d-3} - 2^{b+a-3} - 2^{b-2} < 0.
 \end{aligned} \tag{45}$$

These imply that, if H_4 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_4$, then we infer $0 \leq c - b \leq 1$.

If $c - d \geq 2$, then we have

$$\begin{aligned}
 f_4(a, b, c-1, d+1) - f_4(a, b, c, d) &= 2^{a+b+d-3} - 2^{a+b+c-4} + 2^{b+d-2} - 2^{b+c-3} \\
 &\leq 2^{a+b+c-2-3} - 2^{a+b+c-4} + 2^{b+c-2-2} - 2^{b+c-3} \\
 &= -2^{a+b+c-5} - 2^{b+c-4} < 0.
 \end{aligned} \tag{46}$$

If $d - c \geq 2$, then we have

$$\begin{aligned}
 f_4(a, b, c+1, d-1) - f_4(a, b, c, d) &= -2^{a+b+d-4} + 2^{a+b+c-3} - 2^{b+d-3} + 2^{b+c-2} \\
 &\leq -2^{a+b+c+2-4} + 2^{a+b+c-3} - 2^{b+c+2-3} + 2^{b+c-2} \\
 &= -2^{a+b+c-3} - 2^{b+c-2} < 0.
 \end{aligned} \tag{47}$$

These imply that, if H_4 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_4$, then we infer $|c - d| \leq 1$.

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

$$\begin{aligned}
 f_4(a-1, b, c, d+1) - f_4(a, b, c, d) &= -2^{a+b+c-4} + 2^{b+c+d-2} + 2^{b+d-2} - 2^{b+a-3} \\
 &\leq -2^{d+2+b+c-4} + 2^{b+c+d-2} + 2^{b+d-2} - 2^{b+d+2-3} \\
 &= -2^{b+d-2} < 0.
 \end{aligned} \tag{48}$$

If $d - a \geq 1$, then we have

$$\begin{aligned}
 f_4(a+1, b, c, d-1) - f_4(a, b, c, d) &= 2^{a+b+c-3} - 2^{b+c+d-3} - 2^{b+d-3} + 2^{b+a-2} \\
 &\leq 2^{a+b+c-3} - 2^{b+c+a+1-3} - 2^{b+a+1-3} + 2^{b+a-2} \\
 &= -2^{a+b+c-3} < 0.
 \end{aligned} \tag{49}$$

These imply that, if H_4 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_4$, then we infer $0 \leq a - d \leq 1$. Obviously, as $f_4(a, b, c, d) = f_4(a, b, d, c)$, we can get $0 \leq a - c \leq 1$.

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

$$\begin{aligned} & f_4(a, b+1, c, d-1) - f_4(a, b, c, d) \\ &= 2^{a+c+b-3} - 2^{a+c+d-3} + 2^{b+a-2} + 2^{b+c-2} + 2^{b-1} \\ &\leq 2^{a+c+b-3} - 2^{a+c+b+2-3} + 2^{b+a-2} + 2^{b+c-2} + 2^{b-1} \\ &= 2^{b-1} \left[(1 - 2^{c+a-1}) + 2^{a-1}(1 - 2^{c-1}) + 2^{c-1}(1 - 2^{a-1}) \right] < 0. \end{aligned} \quad (50)$$

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

$$\begin{aligned} & f_4(a, b-1, c, d+1) - f_4(a, b, c, d) \\ &= -2^{a+c+b-4} + 2^{a+c+d-2} - 2^{b+a-3} - 2^{b+c-3} - 2^{b-2} \\ &\leq -2^{a+c+b-4} + 2^{a+c+b-2-2} - 2^{b+a-3} - 2^{b+c-3} - 2^{b-2} \\ &= -2^{b+a-3} - 2^{b+c-3} - 2^{b-2} < 0. \end{aligned} \quad (51)$$

These imply that, if H_4 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_4$, then we infer $|d - b| \leq 1$.

Let $\mathcal{V}_5$ be the set of unicyclic graphs of the form H_5 (as depicted in Figure 9), where v_1, v_2, v_5 , and v_6 are four vertices with $b-1, c-1, d-1$, and $a-1$ pendent vertices, $a+b+c+d = n-2$, $a \geq 2, b, c$, and $d \geq 1$. Let graph H_5^* be the graph of the form H_5 , satisfying $0 \leq a - b \leq 2, -1 \leq c - b \leq 2, -1 \leq d - b \leq 2, |c - d| \leq 1, 0 \leq a - c \leq 1$, and $0 \leq a - d \leq 1$.

Theorem 10. *The graph H_5^* has the minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_5$.*

Proof. Assume $H_5 \in \mathcal{V}_5$. By Lemmas 1 and 2, we get

$$\begin{aligned} i(H_5) &= i(H_5 - \{v_1\}) + i(H_5 - [v_1]) \\ &= i(P_1)^{b-1} i(S_a) [i(S_c) i(S_{d+1}) + i(P_1)^{c-1} i(S_d)] \\ &\quad + i(P_2) i(P_1)^{a+c+d-3} \\ &= 2^{b-1} (2^{a-1} + 1) [(2^{c-1} + 1)(2^d + 1) + 2^{c-1} (2^{d-1} + 1)] \\ &\quad + 3 \cdot 2^{a+c+d-3} \\ &= 3 \cdot 2^{n-6} + 2^{a+b+d-2} + 2^{a+b+c-2} + 3 \cdot 2^{b+c+d-3} \\ &\quad + 3 \cdot 2^{a+c+d-3} + 2^{a+b-2} + 2^{b+c-1} + 2^{b+d-1} + 2^{b-1} \\ &:= f_5(a, b, c, d). \end{aligned} \quad (52)$$

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

FIGURE 9: Unicyclic graphs with diameter three H_5 .

$$\begin{aligned} & f_5(a-1, b+1, c, d) - f_5(a, b, c, d) \\ &= 3 \cdot 2^{b+c+d-3} - 3 \cdot 2^{a+c+d-4} + 2^{b+c-1} + 2^{b+d-1} + 2^{b-1} \\ &\leq 3 \cdot 2^{b+c+d-3} - 3 \cdot 2^{b+3+c+d-4} + 2^{b+c-1} + 2^{b+d-1} + 2^{b-1} \\ &= 2^{b-1} [(1 - 2^{c+d-2}) + 2^d (1 - 2^c) + 2^c (1 - 2^d)] < 0. \end{aligned} \quad (53)$$

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

$$\begin{aligned} & f_5(a+1, b-1, c, d) - f_5(a, b, c, d) \\ &= -3 \cdot 2^{b+c+d-4} + 3 \cdot 2^{a+c+d-3} - 2^{b+c-2} - 2^{b+d-2} - 2^{b-2} \\ &\leq -3 \cdot 2^{b+c+d-4} + 3 \cdot 2^{b-1+c+d-3} - 2^{b+c-2} - 2^{b+d-2} - 2^{b-2} \\ &= -2^{b+c-2} - 2^{b+d-2} - 2^{b-2} < 0. \end{aligned} \quad (54)$$

These imply that, if H_5 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_5$, then we infer $0 \leq a - b \leq 2$.

If $c - b \geq 3$, then we have

$$\begin{aligned} & f_5(a, b+1, c-1, d) - f_5(a, b, c, d) \\ &= 2^{a+b+d-2} - 3 \cdot 2^{a+c+d-4} + 2^{b+a-2} + 2^{b+d-1} + 2^{b-1} \\ &\leq 2^{a+b+d-2} - 3 \cdot 2^{a+b+3+d-4} + 2^{b+a-2} + 2^{b+d-1} + 2^{b-1} \\ &= 2^{b-1} [(1 - 2^{a+d}) + 2^{a-1} (1 - 2^{d+2}) + 2^d (1 - 2^{a+1})] < 0. \end{aligned} \quad (55)$$

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

$$\begin{aligned} & f_5(a, b-1, c+1, d) - f_5(a, b, c, d) \\ &= -2^{a+b+d-3} + 3 \cdot 2^{a+c+d-3} - 2^{b+d-2} - 2^{b+a-3} - 2^{b-2} \\ &\leq -2^{a+b+d-3} + 3 \cdot 2^{a+b-2+d-3} - 2^{b+d-2} - 2^{b+a-3} - 2^{b-2} \\ &= -2^{a+b+d-5} - 2^{b+d-2} - 2^{b+a-3} - 2^{b-2} < 0. \end{aligned} \quad (56)$$

These imply that, if H_5 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_5$, then we infer $-1 \leq c - b \leq 2$. Obviously, as $f_5(a, b, c, d) = f_5(a, b, d, c)$, we can get $-1 \leq d - b \leq 2$.

If $c - d \geq 2$, then we have

$$\begin{aligned}
& f_5(a, b, c-1, d+1) - f_5(a, b, c, d) \\
&= 2^{a+b+d-2} - 2^{a+b+c-3} + 2^{b+d-1} - 2^{b+c-2} \\
&\leq 2^{a+b+d-2} - 2^{a+b+d+2-3} + 2^{b+d-1} - 2^{b+d+2-2} \\
&= -2^{a+b+d-2} - 2^{b+d-1} < 0.
\end{aligned} \tag{57}$$

If $d - c \geq 2$, then we have

$$\begin{aligned}
& f_5(a, b, c+1, d-1) - f_5(a, b, c, d) \\
&= -2^{a+b+d-3} + 2^{a+b+c-2} - 2^{b+d-2} + 2^{b+c-1} \\
&\leq -2^{a+b+c+2-3} + 2^{a+b+c-2} - 2^{b+c+2-2} + 2^{b+c-1} \\
&= -2^{a+b+c-2} - 2^{b+c-1} < 0.
\end{aligned} \tag{58}$$

These imply that, if H_5 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_5$, then we infer $|c - d| \leq 1$.

If $c - a \geq 1$, then we have

$$\begin{aligned}
& f_5(a+1, b, c-1, d) - f_5(a, b, c, d) \\
&= 2^{a+b+d-2} - 3 \cdot 2^{b+c+d-4} + 2^{a+b-1} - 2^{b+c-2} \\
&\leq 2^{a+b+d-2} - 3 \cdot 2^{b+a+1+d-4} + 2^{a+b-1} - 2^{b+a+1-2} \\
&= -2^{a+b+d-3} < 0.
\end{aligned} \tag{59}$$

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

$$\begin{aligned}
& f_5(a-1, b, c+1, d) - f_5(a, b, c, d) \\
&= -2^{a+b+d-3} + 3 \cdot 2^{b+c+d-3} - 2^{a+b-3} + 2^{b+c-1} \\
&\leq -2^{c+2+b+d-3} + 3 \cdot 2^{b+c+d-3} - 2^{c+2+b-3} + 2^{b+c-1} \\
&= -2^{b+c+d-3} < 0.
\end{aligned} \tag{60}$$

These imply that, if H_5 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_5$, then we infer $0 \leq a - c \leq 1$. Obviously, as $f_5(a, b, c, d) = f_5(a, b, d, c)$, we can get $0 \leq a - d \leq 1$.

Let $\mathcal{V}_6$ be the set of unicyclic graphs of the form H_6 (as depicted in Figure 10), 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, $a+b+c+d+e = n$, a, b, c, d , and $e \geq 1$. As the diameter is 4, from symmetry, we may assume a and c , or a and d , are at least 2. Let graph H_6^* be the graph of the form H_6 , satisfying a, b, c, d , and e almost equal, that is, $\forall x, y \in \{a, b, c, d, e\}$, $x \neq y$, and $|x - y| \leq 1$.

Theorem 11. *The graph H_6^* has the minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_6$.*

Proof. Assume $H_6 \in \mathcal{V}_6$. By Lemmas 1 and 2, we get

FIGURE 10: Unicyclic graphs with diameter three H_6 .

$$\begin{aligned}
i(H_6) &= i(H_6 - \{v_1\}) + i(H_6 - [v_1]) \\
&= i(P_1)^{a-1} \{i(P_1)^{c-1} i(S_b) [i(P_1)^{d-1} i(S_e) + i(P_1)^{e-1}] \\
&\quad + i(P_1)^{b+d-2} i(S_e)\} + i(P_1)^{b+e-2} [i(P_1)^{c-1} i(S_d) + i(P_1)^{d-1}] \\
&= 2^{a-1} \{2^{c-1} (2^{b-1} + 1) [2^{d-1} (2^{e-1} + 1) + 2^{e-1}] \\
&\quad + 2^{b+d-2} (2^{e-1} + 1)\} + 2^{b+e-2} [2^{c-1} (2^{d-1} + 1) + 2^{d-1}] \\
&= 2^{n-5} + 2^{a+b+c+d-4} + 2^{a+b+c+e-4} + 2^{a+c+d+e-4} + 2^{a+b+d+e-4} \\
&\quad + 2^{b+c+d+e-4} + 2^{a+c+d-3} + 2^{a+c+e-3} + 2^{a+b+d-3} \\
&\quad + 2^{b+c+e-3} + 2^{b+d+e-3} := f_6(a, b, c, d, e).
\end{aligned} \tag{61}$$

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

$$\begin{aligned}
& f_6(a-1, b+1, c, d, e) - f_6(a, b, c, d, e) \\
&= -2^{a+c+d+e-5} + 2^{b+c+d+e-4} - 2^{a+c+d-4} - 2^{a+c+e-4} \\
&\quad + 2^{b+c+e-3} + 2^{b+d+e-3} \\
&\leq -2^{b+2+c+d+e-5} + 2^{b+c+d+e-4} - 2^{b+2+c+d-4} - 2^{b+2+c+e-4} \\
&\quad + 2^{b+c+e-3} + 2^{b+d+e-3} \\
&= -3 \cdot 2^{b+c+e-3} + 2^{b+d+e-3} (1 - 2^{c-1}) < 0.
\end{aligned} \tag{62}$$

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

$$\begin{aligned}
& f_6(a+1, b-1, c, d, e) - f_6(a, b, c, d, e) \\
&= 2^{a+c+d+e-4} - 2^{b+c+d+e-5} + 2^{a+c+d-3} + 2^{a+c+e-3} \\
&\quad - 2^{b+c+e-4} - 2^{b+d+e-4} \\
&\leq 2^{a+c+d+e-4} - 2^{a+2+c+d+e-5} + 2^{a+c+d-3} + 2^{a+c+e-3} \\
&\quad - 2^{a+2+c+e-4} - 2^{a+2+d+e-4} \\
&= -2^{a+c+d+e-4} + 2^{a+c+d-3} - 2^{a+c+e-3} - 2^{a+d+e-2} \\
&= 2^{a+c+d-3} (1 - 2^{e-1}) - 2^{a+c+e-3} - 2^{a+d+e-2} < 0.
\end{aligned} \tag{63}$$

These imply that, if H_6 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_6$, then we infer $|a - b| \leq 1$.

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

$$\begin{aligned}
& f_6(a, b-1, c+1, d, e) - f_6(a, b, c, d, e) \\
&= 2^{a+c+d+e-4} - 2^{a+b+d+e-5} - 2^{a+b+d-4} - 2^{b+d+e-4} \\
&\quad + 2^{a+c+d-3} + 2^{a+c+e-3} \\
&\leq 2^{a+b-2+d+e-4} - 2^{a+b+d+e-5} - 2^{a+b+d-4} - 2^{b+d+e-4} \quad (64) \\
&\quad + 2^{a+b-2+d-3} + 2^{a+b-2+e-3} \\
&= -2^{b+d+e-4} - 2^{a+d+b-5} + 2^{a+b+e-5}(1-2^{d-1}) < 0.
\end{aligned}$$

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

$$\begin{aligned}
& f_6(a, b+1, c-1, d, e) - f_6(a, b, c, d, e) \\
&= -2^{a+c+d+e-5} + 2^{a+b+d+e-4} + 2^{a+b+d-3} + 2^{b+d+e-3} \\
&\quad - 2^{a+c+d-4} - 2^{a+c+e-4} \\
&\leq -2^{a+b+2+d+e-5} + 2^{a+b+d+e-4} + 2^{a+b+d-3} + 2^{b+d+e-3} \\
&\quad - 2^{a+b+2+d-4} - 2^{a+b+2+e-4} \\
&= -2^{a+b+e-2} - 2^{a+b+d-3} + 2^{b+e+d-3}(1-2^{a-1}) < 0. \quad (65)
\end{aligned}$$

These imply that, if H_6 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_6$, then we infer $|c-b| \leq 1$.

If $c-d \geq 2$, then we have

$$\begin{aligned}
& f_6(a, b, c-1, d+1, e) - f_6(a, b, c, d, e) \\
&= -2^{a+b+c+e-5} + 2^{a+b+d+e-4} - 2^{a+c+e-4} - 2^{b+c+e-4} \\
&\quad + 2^{a+b+d-3} + 2^{b+d+e-3} \\
&\leq -2^{a+b+d+2+e-5} + 2^{a+b+d+e-4} - 2^{a+d+2+e-4} - 2^{b+d+2+e-4} \\
&\quad + 2^{a+b+d-3} + 2^{b+d+e-3} \\
&= -2^{b+d+e-3} - 2^{a+d+e-2} + 2^{a+b+d-3}(1-2^{e-1}) < 0. \quad (66)
\end{aligned}$$

If $d-c \geq 2$, then we have

$$\begin{aligned}
& f_6(a, b, c+1, d-1, e) - f_6(a, b, c, d, e) \\
&= 2^{a+b+c+e-4} - 2^{a+b+d+e-5} + 2^{a+c+e-3} + 2^{b+c+e-3} \\
&\quad - 2^{a+b+d-4} - 2^{b+d+e-4} \\
&\leq 2^{a+b+d-2+e-4} - 2^{a+b+d+e-5} + 2^{a+d-2+e-3} + 2^{b+d-2+e-3} \\
&\quad - 2^{a+b+d-4} - 2^{b+d+e-4} \\
&= -2^{b+d+e-5} - 2^{a+b+d-4} + 2^{a+e+d-5}(1-2^{b-1}) < 0. \quad (67)
\end{aligned}$$

These imply that, if H_6 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_6$, then we infer $|c-d| \leq 1$.

If $e-d \geq 2$, then we have

$$\begin{aligned}
& f_6(a, b, c, d+1, e-1) - f_6(a, b, c, d, e) \\
&= 2^{a+b+c+d-4} - 2^{a+b+c+e-5} + 2^{a+c+d-3} + 2^{a+b+d-3} \\
&\quad - 2^{a+c+e-4} - 2^{b+c+e-4} \\
&\leq 2^{a+b+c+e-2-4} - 2^{a+b+c+e-5} + 2^{a+c+e-2-3} + 2^{a+b+e-2-3} \\
&\quad - 2^{a+c+e-4} - 2^{b+c+e-4} \\
&= -2^{b+c+e-4} - 2^{a+c+e-5} + 2^{a+b+e-5}(1-2^{c-1}) < 0. \quad (68)
\end{aligned}$$

If $d-e \geq 2$, then we have

$$\begin{aligned}
& f_6(a, b, c, d-1, e+1) - f_6(a, b, c, d, e) \\
&= -2^{a+b+c+d-5} + 2^{a+b+c+e-4} - 2^{a+c+d-4} - 2^{a+b+d-4} \\
&\quad + 2^{a+c+e-3} + 2^{b+c+e-3} \\
&\leq -2^{a+b+c+e+2-5} + 2^{a+b+c+e-4} - 2^{a+c+e+2-4} - 2^{a+b+e+2-4} \\
&\quad + 2^{a+c+e-3} + 2^{b+c+e-3} \\
&= -2^{a+c+e-3} - 2^{a+b+e-2} + 2^{b+c+e-3}(1-2^{a-1}) < 0. \quad (69)
\end{aligned}$$

These imply that, if H_6 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_6$, then we infer $|e-d| \leq 1$.

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

$$\begin{aligned}
& f_6(a+1, b, c, d, e-1) - f_6(a, b, c, d, e) \\
&= 2^{a+b+c+d-4} - 2^{b+c+d+e-5} + 2^{a+c+d-3} + 2^{a+b+d-3} \\
&\quad - 2^{b+c+e-4} - 2^{b+d+e-4} \\
&\leq 2^{e-2+b+c+d-4} - 2^{b+c+d+e-5} + 2^{e-2+c+d-3} + 2^{e-2+b+d-3} \\
&\quad - 2^{b+c+e-4} - 2^{b+d+e-4} \\
&= -2^{b+c+e-4} - 2^{b+d+e-5} + 2^{e+c+d-5}(1-2^{b-1}) < 0. \quad (70)
\end{aligned}$$

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

$$\begin{aligned}
& f_6(a-1, b, c, d, e+1) - f_6(a, b, c, d, e) \\
&= -2^{a+b+c+d-5} + 2^{b+c+d+e-4} - 2^{a+c+d-4} - 2^{a+b+d-4} \\
&\quad + 2^{b+c+e-3} + 2^{b+d+e-3} \\
&\leq -2^{e+2+b+c+d-5} + 2^{b+c+d+e-4} - 2^{e+2+c+d-4} - 2^{e+2+b+d-4} \\
&\quad + 2^{b+c+e-3} + 2^{b+d+e-3} \\
&= -2^{c+d+e-2} - 2^{b+d+e-3} + 2^{e+c+b-3}(1-2^{d-1}) < 0. \quad (71)
\end{aligned}$$

These imply that, if H_6 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_6$, then we infer $|e-a| \leq 1$.

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

$$\begin{aligned}
& f_6(a-1, b, c+1, d, e) - f_6(a, b, c, d, e) \\
&= -2^{a+b+d+e-5} + 2^{b+c+d+e-4} - 2^{a+b+d-4} + 2^{b+c+e-3} \\
&\leq -2^{c+2+b+d+e-5} + 2^{b+c+d+e-4} - 2^{c+2+b+d-4} + 2^{b+c+e-3} \\
&= -2^{b+c+d-2} + 2^{b+c+e-3}(1 - 2^{d-1}) < 0.
\end{aligned} \tag{72}$$

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

$$\begin{aligned}
& f_6(a+1, b, c-1, d, e) - f_6(a, b, c, d, e) \\
&= 2^{a+b+d+e-4} - 2^{b+c+d+e-5} + 2^{a+b+d-3} - 2^{b+c+e-4} \\
&\leq 2^{a+b+d+e-4} - 2^{b+a+2+d+e-5} + 2^{a+b+d-3} - 2^{b+a+2+e-4} \\
&= -2^{a+b+e-2} + 2^{a+b+d-3}(1 - 2^{e-1}) < 0.
\end{aligned} \tag{73}$$

These imply that, if H_6 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_6$, then we infer $|a - c| \leq 1$.

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

$$\begin{aligned}
& f_6(a, b-1, c, d+1, e) - f_6(a, b, c, d, e) \\
&= -2^{a+b+c+e-5} + 2^{a+d+c+e-4} + 2^{a+c+d-3} - 2^{c+b+e-4} \\
&\leq -2^{a+d+2+c+e-5} + 2^{a+d+c+e-4} + 2^{a+c+d-3} - 2^{c+d+2+e-4} \\
&= -2^{d+c+e-2} + 2^{a+c+d-3}(1 - 2^{e-1}) < 0.
\end{aligned} \tag{74}$$

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

$$\begin{aligned}
& f_6(a, b+1, c, d-1, e) - f_6(a, b, c, d, e) \\
&= 2^{a+b+c+e-4} - 2^{a+d+c+e-5} - 2^{a+c+d-4} + 2^{c+b+e-3} \\
&\leq 2^{a+b+c+e-4} - 2^{a+b+2+c+e-5} - 2^{a+c+b+2-4} + 2^{c+b+e-3} \\
&= -2^{a+b+c-2} + 2^{b+c+e-3}(1 - 2^{a-1}) < 0.
\end{aligned} \tag{75}$$

These imply that, if H_6 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_6$, then we infer $|b - d| \leq 1$.

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

$$\begin{aligned}
& f_6(a-1, b, c, d+1, e) - f_6(a, b, c, d, e) \\
&= -2^{a+b+c+e-5} + 2^{b+d+c+e-4} + 2^{b+e+d-3} - 2^{c+a+e-4} \\
&\leq -2^{d+2+b+c+e-5} + 2^{b+d+c+e-4} + 2^{b+e+d-3} - 2^{c+d+2+e-4} \\
&= -2^{d+c+e-2} + 2^{b+e+d-3}(1 - 2^{c-1}) < 0.
\end{aligned} \tag{76}$$

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

$$\begin{aligned}
& f_6(a+1, b, c, d-1, e) - f_6(a, b, c, d, e) \\
&= 2^{a+b+c+e-4} - 2^{b+d+c+e-5} - 2^{b+e+d-4} + 2^{c+a+e-3} \\
&\leq 2^{a+b+c+e-4} - 2^{b+a+2+c+e-5} - 2^{b+e+a+2-4} + 2^{c+a+e-3} \\
&= -2^{a+b+e-2} + 2^{a+e+c-3}(1 - 2^{b-1}) < 0.
\end{aligned} \tag{77}$$

These imply that, if H_6 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_6$, then we infer $|a - d| \leq 1$.

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

$$\begin{aligned}
& f_6(a, b+1, c, d, e-1) - f_6(a, b, c, d, e) \\
&= 2^{a+b+c+d-4} - 2^{a+c+d+e-5} + 2^{a+b+d-3} - 2^{a+c+e-4} \\
&\leq 2^{a+b+c+d-4} - 2^{a+c+d+b+2-5} + 2^{a+b+d-3} - 2^{a+c+b+2-4} \\
&= -2^{b+c+a-2} + 2^{a+b+d-3}(1 - 2^{c-1}) < 0.
\end{aligned} \tag{78}$$

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

$$\begin{aligned}
& f_6(a, b-1, c, d, e+1) - f_6(a, b, c, d, e) \\
&= -2^{a+b+c+d-5} + 2^{a+c+d+e-4} - 2^{a+b+d-4} + 2^{a+c+e-3} \\
&\leq -2^{a+e+2+c+d-5} + 2^{a+c+d+e-4} - 2^{a+e+2+d-4} + 2^{a+c+e-3} \\
&= -2^{d+e+a-2} + 2^{a+c+e-3}(1 - 2^{d-1}) < 0.
\end{aligned} \tag{79}$$

These imply that, if H_6 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_6$, then we infer $|e - b| \leq 1$.

If $e - c \geq 2$, then we have

$$\begin{aligned}
& f_6(a, b, c+1, d, e-1) - f_6(a, b, c, d, e) \\
&= 2^{a+b+c+d-4} - 2^{a+b+d+e-5} + 2^{a+c+d-3} - 2^{b+d+e-4} \\
&\leq 2^{a+b+c+d-4} - 2^{a+b+d+c+2-5} + 2^{a+c+d-3} - 2^{b+d+c+2-4} \\
&= -2^{b+c+d-2} + 2^{a+c+d-3}(1 - 2^{b-1}) < 0.
\end{aligned} \tag{80}$$

If $c - e \geq 2$, then we have

$$\begin{aligned}
& f_6(a, b, c-1, d, e+1) - f_6(a, b, c, d, e) \\
&= -2^{a+b+c+d-5} + 2^{b+a+d+e-4} - 2^{a+c+d-4} + 2^{e+b+d-3} \\
&\leq -2^{a+b+e+2+d-5} + 2^{b+a+d+e-4} - 2^{a+e+2+d-4} + 2^{e+b+d-3} \\
&= -2^{a+d+e-2} + 2^{e+d+b-3}(1 - 2^{a-1}) < 0.
\end{aligned} \tag{81}$$

These imply that, if H_6 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_6$, then we infer $|e - c| \leq 1$.

Let $\mathcal{V}_7$ be the set of unicyclic graphs of the form H_7 (as depicted in Figure 11), 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 , and $c \geq 1$, and one of a, b , and c is at least 2. Let graph H_7^* be the graph of the form H_7 , satisfying a, b , and c almost equal, that is, $|a - b| \leq 1$, $|b - c| \leq 1$, and $|c - a| \leq 1$.

Theorem 12. *The graph H_7^* has the minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_7$.*

Proof. Assume $H_7 \in \mathcal{V}_7$. By Lemmas 1 and 2, we get

FIGURE 11: Unicyclic graphs with diameter three H_7 .

$$\begin{aligned}
 i(H_7) &= i(H_7 - \{v_1\}) + i(H_7 - [v_1]) \\
 &= i(P_1)^{a-1} [i(P_3)i(P_1)^{c-1}i(S_b) + i(P_1)^{b-1}i(P_2)] \\
 &\quad + i(P_1)^{b-1} [i(P_2)i(P_1)^{c-1} + i(P_1)] \\
 &= 2^{a-1} [5 \cdot 2^{c-1}(2^{b-1} + 1) + 3 \cdot 2^{b-1}] + 2^{b-1} [3 \cdot 2^{c-1} + 2] \\
 &= 5 \cdot 2^{n-6} + 5 \cdot 2^{a+c-2} + 3 \cdot 2^{a+b-2} + 3 \cdot 2^{b+c-2} + 2^b \\
 &:= f_7(a, b, c).
 \end{aligned} \tag{82}$$

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

$$\begin{aligned}
 f_7(a-1, b+1, c) - f_7(a, b, c) \\
 &= -5 \cdot 2^{a+c-3} + 3 \cdot 2^{b+c-2} + 2^b \\
 &\leq -5 \cdot 2^{b+2+c-3} + 3 \cdot 2^{b+c-2} + 2^b \\
 &= 2^b(1 - 7 \cdot 2^{c-2}) < 0.
 \end{aligned} \tag{83}$$

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

$$\begin{aligned}
 f_7(a+1, b-1, c) - f_7(a, b, c) \\
 &= 5 \cdot 2^{a+c-2} - 3 \cdot 2^{b+c-3} - 2^{b-1} \\
 &\leq 5 \cdot 2^{b-2+c-2} - 3 \cdot 2^{b+c-3} - 2^{b-1} \\
 &= -2^{b+c-4} - 2^{b-1} < 0.
 \end{aligned} \tag{84}$$

These imply that, if H_7 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_7$, then we infer $|a - b| \leq 1$. Obviously, as $f_7(a, b, c) = f_7(c, b, a)$, we can get $|c - b| \leq 1$.

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

$$\begin{aligned}
 f_7(a-1, b, c+1) - f_7(a, b, c) \\
 &= -3 \cdot 2^{b+a-3} + 3 \cdot 2^{b+c-2} \\
 &\leq -3 \cdot 2^{b+c+2-3} + 3 \cdot 2^{b+c-2} \\
 &= -3 \cdot 2^{b+c-2} < 0.
 \end{aligned} \tag{85}$$

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

$$\begin{aligned}
 f_7(a+1, b, c-1) - f_7(a, b, c) \\
 &= 3 \cdot 2^{b+a-2} - 3 \cdot 2^{b+c-3} \\
 &\leq 3 \cdot 2^{b+c-2-2} - 3 \cdot 2^{b+c-3} \\
 &= -3 \cdot 2^{b+c-4} < 0.
 \end{aligned} \tag{86}$$

These imply that, if H_7 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_7$, then we infer $|a - c| \leq 1$.

Let $\mathcal{V}_8$ be the set of unicyclic graphs of the form H_8 (as depicted in Figure 12), 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 , and $c \geq 1$, and one of a, b , and c is at least 2. Let graph H_8^* be the graph of the form H_8 , satisfying a, b , and c almost equal, that is, $|a - b| \leq 1$, $|b - c| \leq 1$, and $|c - a| \leq 1$.

Theorem 13. *The graph H_8^* has the minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_8$.*

Proof. Assume $H_8 \in \mathcal{V}_8$. By Lemmas 1 and 2, we get

$$\begin{aligned}
 i(H_8) &= i(H_8 - \{v_1\}) + i(H_8 - [v_1]) \\
 &= i(P_1)^{a-1} [i(P_4)i(P_1)^{c-1}i(S_b) + i(P_1)^{b-1}i(P_3)] \\
 &\quad + i(P_1)^{b-1} [i(P_3)i(P_1)^{c-1} + i(P_2)] \\
 &= 2^{a-1} [8 \cdot 2^{c-1}(2^{b-1} + 1) + 5 \cdot 2^{b-1}] + 2^{b-1} [5 \cdot 2^{c-1} + 3] \\
 &= 2^{n-4} + 2^{a+c+1} + 5 \cdot 2^{a+b-2} + 5 \cdot 2^{b+c-2} + 3 \cdot 2^{b-1} \\
 &:= f_8(a, b, c).
 \end{aligned} \tag{87}$$

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

$$\begin{aligned}
 f_8(a-1, b+1, c) - f_8(a, b, c) \\
 &= -2^{a+c} + 5 \cdot 2^{b+c-2} + 3 \cdot 2^{b-1} \\
 &\leq -2^{b+2+c} + 5 \cdot 2^{b+c-2} + 3 \cdot 2^{b-1} \\
 &= 2^{b-1}(3 - 11 \cdot 2^{c-1}) < 0.
 \end{aligned} \tag{88}$$

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

$$\begin{aligned}
 f_8(a+1, b-1, c) - f_8(a, b, c) \\
 &= 2^{a+c+1} - 5 \cdot 2^{b+c-3} - 3 \cdot 2^{b-2} \\
 &\leq 2^{b-2+c+1} - 5 \cdot 2^{b+c-3} - 3 \cdot 2^{b-2} \\
 &= -2^{b+c-3} - 3 \cdot 2^{b-2} < 0.
 \end{aligned} \tag{89}$$

These imply that, if H_8 has minimum Merri-field-Simmons index among all graphs in $\mathcal{V}_8$, then we infer $|a - b| \leq 1$. Obviously, as $f_8(a, b, c) = f_8(c, b, a)$, we can get $|c - b| \leq 1$.

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

$$\begin{aligned}
 f_8(a-1, b, c+1) - f_8(a, b, c) \\
 &= -5 \cdot 2^{b+a-3} + 5 \cdot 2^{b+c-2} \\
 &\leq -5 \cdot 2^{b+a-3} + 5 \cdot 2^{b+a-2-2} \\
 &= -5 \cdot 2^{b+a-4} < 0.
 \end{aligned} \tag{90}$$

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

FIGURE 12: Unicyclic graphs with diameter three H_8 .

$$\begin{aligned}
 & f_8(a+1, b, c-1) - f_8(a, b, c) \\
 &= 5 \cdot 2^{b+a-2} - 5 \cdot 2^{b+c-3} \\
 &\leq 5 \cdot 2^{b+a-2} - 5 \cdot 2^{b+a+2-3} \\
 &= -5 \cdot 2^{b+a-2} < 0.
 \end{aligned} \tag{91}$$

These imply that, if H_8 has minimum Merrifield-Simmons index among all graphs in $\mathcal{V}_8$, then we infer $|a - c| \leq 1$.

Let $\mathcal{V}_9$ be the set of unicyclic graphs of the form H_9 (as depicted in Figure 13), 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 , and $c \geq 1$, and one of a, b , and c is at least 2. Let graph H_9^* be the graph of the form H_9 , satisfying a, b , and c almost equal, that is, $|a - b| \leq 1$, $|b - c| \leq 1$, and $|c - a| \leq 1$.

Theorem 14. *The graph H_9^* has the minimum Merrifield-Simmons index among all graphs in $\mathcal{V}_9$.*

Proof. Assume $H_9 \in \mathcal{V}_9$. By Lemmas 1 and 2, we get

$$\begin{aligned}
 i(H_9) &= i(H_9 - \{v_1\}) + i(H_9 - [v_1]) \\
 &= i(P_1)^{a-1} [i(S_{c+1})i(S_{b+1}) + i(P_1)^{b+c}] \\
 &\quad + i(S_c)i(S_b) + i(P_1)^{b+c-2} \\
 &= 2^{a-1} [(2^c + 1)(2^b + 1) + 2^{b+c}] \\
 &\quad + (2^{c-1} + 1)(2^{b-1} + 1) + 2^{b+c-2} \\
 &= 2^{n-3} + 2^{a+b-1} + 2^{b+c-1} + 2^{a+c-1} + 2^{a-1} \\
 &\quad + 2^{b-1} + 2^{c-1} + 1 \\
 &:= f_9(a, b, c).
 \end{aligned} \tag{92}$$

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

$$\begin{aligned}
 & f_9(a-1, b+1, c) - f_9(a, b, c) \\
 &= 2^{b+c-1} - 2^{a+c-2} - 2^{a-2} + 2^{b-1} \\
 &\leq 2^{a-2+c-1} - 2^{a+c-2} - 2^{a-2} + 2^{a-2-1} \\
 &= -2^{a+c-3} - 2^{a-3} < 0.
 \end{aligned} \tag{93}$$

FIGURE 13: Unicyclic graphs with diameter three H_9 .

Obviously, a, b , and c have the same status in $f_9(a, b, c)$. Thus, if H_9 has minimum Merrifield-Simmons index among all graphs in $\mathcal{V}_9$, then we infer $|a - b| \leq 1$; further, $|b - c| \leq 1$ and $|c - a| \leq 1$. This is the above desired result.

Theorem 15. *The graph H_6^* has the minimum Merrifield-Simmons index among all graphs in $\mathcal{V}_n^4$ if $n \geq 29$.*

Proof. We only need to compare the Merrifield-Simmons indices of H_i^* for $i = 1, 2, 3, 4, 5, 6, 7, 8, 9$.

For H_1^* , as $0 \leq a - b \leq 1$ and $0 \leq a - c \leq 2$, we have $b \leq a \leq b+1$ and $c \leq a \leq c+2$. Since $a+b+c = n-2$, we get $a \geq (n-2/3)$. Therefore,

$$\begin{aligned}
 i(H_1^*) &= 3 \cdot 2^{n-5} + 3 \cdot 2^{a+c-2} + 3 \cdot 2^{b+c-2} + 2^{b+a-2} + 2^{b-1} \\
 &\geq 3 \cdot 2^{n-5} + 3 \cdot 2^{2a-4} + 3 \cdot 2^{2a-5} + 2^{2a-3} + 2^{a-2} \\
 &= 3 \cdot 2^{n-5} + 13 \cdot 2^{2a-5} + 2^{a-2} \\
 &\geq 3 \cdot 2^{n-5} + 13 \cdot 2^{(2n-19/3)} + 2^{(n-8/3)} := g_1(n).
 \end{aligned} \tag{94}$$

For H_2^* , as $0 \leq a - b \leq 2$, $0 \leq a - d \leq 2$, and $0 \leq a - c \leq 1$, we have $b \leq a \leq b+2$, $c \leq a \leq c+1$, and $d \leq a \leq d+2$. Since $a+b+c+d = n$, we get $a \geq (n/4)$. Therefore,

$$\begin{aligned}
 i(H_2^*) &= 2^{n-4} + 2^{a+c+d-3} + 2^{a+b+d-3} + 2^{b+c+d-3} + 2^{a+b+c-3} \\
 &\quad + 2^{b+d-2} + 2^{b+c-2} \\
 &\geq 2^{n-4} + 11 \cdot 2^{3a-8} + 3 \cdot 2^{2a-6} \\
 &\geq 2^{n-4} + 11 \cdot 2^{(3n-32/4)} + 3 \cdot 2^{(n-12/2)} := g_2(n).
 \end{aligned} \tag{95}$$

For H_3^* , as a, b, c , and d are almost equal, we have $b-1 \leq a \leq b+1$, $c-1 \leq a \leq c+1$, and $d-1 \leq a \leq d+1$. Since $a+b+c+d = n$, we get $a \geq (n-3/4)$. Therefore,

$$\begin{aligned}
 i(H_3^*) &= 2^{n-4} + 2^{a+c+d-3} + 2^{a+b+d-3} + 2^{b+c+d-3} \\
 &\quad + 2^{a+b+c-3} + 2^{b+d-2} + 2^{a+c-2} \\
 &\geq 2^{n-4} + 7 \cdot 2^{3a-6} + 3 \cdot 2^{2a-4} \\
 &\geq 2^{n-4} + 7 \cdot 2^{(3n-33/4)} + 3 \cdot 2^{(n-11/2)} := g_3(n).
 \end{aligned} \tag{96}$$

For H_4^* , as $0 \leq a - b \leq 2$, $0 \leq a - d \leq 1$, and $0 \leq a - c \leq 1$, we have $b \leq a \leq b + 2$, $c \leq a \leq c + 1$, and $d \leq a \leq d + 1$. Since $a + b + c + d = n - 1$, we get $a \geq (n - 1/4)$. Therefore,

$$\begin{aligned} i(H_4^*) &= 2^{n-4} + 2^{a+b+d-3} + 2^{a+b+c-3} + 2^{b+c+d-2} + 2^{a+c+d-2} \\ &\quad + 2^{a+b-2} + 2^{b+c-2} + 2^{b+d-2} + 2^{b-1} \\ &\geq 2^{n-4} + 7 \cdot 2^{3a-6} + 2^{2a-3} + 2^{a-3} \\ &\geq 2^{n-4} + 7 \cdot 2^{(3n-27/4)} + 2^{(n-7/2)} + 2^{(n-13/4)} := g_4(n). \end{aligned} \quad (97)$$

For H_5^* , as $0 \leq a - b \leq 2$, $0 \leq a - c \leq 1$, and $0 \leq a - d \leq 1$, we have $b \leq a \leq b + 2$, $c \leq a \leq c + 1$, and $d \leq a \leq d + 1$. Since $a + b + c + d = n - 2$, we get $a \geq (n - 2/4)$. Therefore,

$$\begin{aligned} i(H_5^*) &= 3 \cdot 2^{n-6} + 2^{a+b+d-2} + 2^{a+b+c-2} + 3 \cdot 2^{b+c+d-3} \\ &\quad + 3 \cdot 2^{a+c+d-3} + 2^{a+b-2} + 2^{b+c-1} + 2^{b+d-1} + 2^{b-1} \\ &\geq 3 \cdot 2^{n-6} + 23 \cdot 2^{3a-7} + 3 \cdot 2^{2a-4} + 2^{a-3} \\ &\geq 3 \cdot 2^{n-6} + 23 \cdot 2^{(3n-34/4)} + 3 \cdot 2^{(n-10/2)} + 2^{(n-14/4)} \\ &:= g_5(n). \end{aligned} \quad (98)$$

For H_6^* , as a, b, c, d , and e are almost equal, we have $b - 1 \leq a \leq b + 1$, $c - 1 \leq a \leq c + 1$, $d - 1 \leq a \leq d + 1$, and $e - 1 \leq a \leq e + 1$. Since $a + b + c + d + e = n$, we get $a \geq (n - 4/5)$. Therefore,

$$\begin{aligned} i(H_6^*) &= 2^{n-5} + 2^{a+b+c+d-4} + 2^{a+b+c+e-4} + 2^{a+c+d+e-4} \\ &\quad + 2^{a+b+d+e-4} + 2^{b+c+d+e-4} + 2^{a+c+d-3} + 2^{a+c+e-3} \\ &\quad + 2^{a+b+d-3} + 2^{b+c+e-3} + 2^{b+d+e-3} \\ &\geq 2^{n-5} + 9 \cdot 2^{4a-8} + 2^{3a-3} \\ &\geq 2^{n-5} + 9 \cdot 2^{(4n-56/5)} + 2^{(3n-27/5)} := g_6(n). \end{aligned} \quad (99)$$

For H_7^* , as a, b , and c are almost equal, we have $b - 1 \leq a \leq b + 1$ and $c - 1 \leq a \leq c + 1$. Since $a + b + c = n - 3$, we get $a \geq (n - 5/3)$. Therefore,

$$\begin{aligned} i(H_7^*) &= 5 \cdot 2^{n-6} + 5 \cdot 2^{a+c-2} + 3 \cdot 2^{a+b-2} + 3 \cdot 2^{b+c-2} + 2^b \\ &\geq 5 \cdot 2^{n-6} + 19 \cdot 2^{2a-4} + 2^{a-1} \\ &\geq 5 \cdot 2^{n-6} + 19 \cdot 2^{(2n-22/3)} + 2^{(n-8/3)} := g_7(n). \end{aligned} \quad (100)$$

For H_8^* , as a, b , and c are almost equal, we have $b - 1 \leq a \leq b + 1$ and $c - 1 \leq a \leq c + 1$. Since $a + b + c = n - 4$, we get $a \geq (n - 6/3)$. Therefore,

$$\begin{aligned} i(H_8^*) &= 2^{n-4} + 2^{a+c+1} + 5 \cdot 2^{a+b-2} + 5 \cdot 2^{b+c-2} + 3 \cdot 2^{b-1} \\ &\geq 2^{n-4} + 31 \cdot 2^{2a-4} + 3 \cdot 2^{a-2} \\ &\geq 2^{n-4} + 31 \cdot 2^{(2n-24/3)} + 3 \cdot 2^{(n-12/3)} := g_8(n). \end{aligned} \quad (101)$$

For H_9^* , as a, b , and c are almost equal, we have $b - 1 \leq a \leq b + 1$ and $c - 1 \leq a \leq c + 1$. Since $a + b + c = n - 3$, we get $a \geq (n - 5/3)$. Therefore,

$$\begin{aligned} i(H_9^*) &= 2^{n-3} + 2^{a+b-1} + 2^{b+c-1} + 2^{a+c-1} + 2^{a-1} \\ &\quad + 2^{b-1} + 2^{c-1} + 1 \geq 2^{n-3} + 5 \cdot 2^{2a-3} + 2^a + 1 \\ &\geq 2^{n-3} + 5 \cdot 2^{(2n-19/3)} + 2^{(n-5/3)} + 1 := g_9(n). \end{aligned} \quad (102)$$

By simple calculation comparison, we obtain the following comparison:

$$\begin{aligned} g_2(n) - g_3(n) &= 2^{(3n-33/4)} (11 \cdot 2^{(1/4)} - 7) \\ &\quad + 3 \cdot 2^{(n-12/2)} (1 - 2^{(1/2)}) \\ &> 3 \cdot 2^{(3n-29/4)} - 3 \cdot 2^{(n-14/2)} \\ &= 3 \cdot 2^{(n-14/2)} (2^{(n-1/4)} - 1) > 0. \end{aligned} \quad (103)$$

Thus, we get $g_2(n) > g_3(n)$, for $n \geq 12$.

$$\begin{aligned} g_4(n) - g_3(n) &= 7 \cdot 2^{(3n-33/4)} (2^{(3/2)} - 1) + 2^{(n-11/2)} (2^2 - 3) \\ &\quad + 2^{(n-13/4)} \\ &> 7 \cdot 2^{(3n-33/4)} + 2^{(n-11/2)} + 2^{(n-13/4)} > 0. \end{aligned} \quad (104)$$

Thus, we get $g_4(n) > g_3(n)$ for $n \geq 13$,

$$\begin{aligned} g_3(n) - g_8(n) &= 2^{(2n-24/3)} (7 \cdot 2^{(n-3/12)} - 31) \\ &\quad + 3 \cdot 2^{(n-12/3)} (2^{(n-9/6)} - 1). \end{aligned} \quad (105)$$

If $n \geq 29$, then $7 \cdot 2^{(n-3/12)} - 31 > 0$ and $2^{(n-9/6)} - 1 > 0$. Thus, we get $g_3(n) > g_8(n)$ for $n \geq 29$.

$$\begin{aligned} g_9(n) - g_8(n) &= 2^{n-4} + 2^{(2n-24/3)} (5 \cdot 2^{(5/3)} - 31) \\ &\quad + 2^{(n-12/3)} (2^{(7/3)} - 3) + 1 \\ &> 2^{n-4} - 2^{(2n-12/3)} + 2^{(n-9/3)} + 1 \\ &= 2^{(2n-12/3)} (2^{(n/3)} - 1) + 2^{(n-9/3)} + 1 > 0. \end{aligned} \quad (106)$$

Thus, we get $g_9(n) > g_8(n)$ for $n \geq 12$.

$$\begin{aligned} g_7(n) - g_8(n) &= 2^{n-6} + 2^{(2n-24/3)} (19 \cdot 2^{(2/3)} - 31) \\ &\quad + 2^{(n-12/3)} (2^{(4/3)} - 3) \\ &= 2^{n-6} - 2^{(2n-24/3)} - 2^{(n-15/3)} \\ &= 2^{(n-15/3)} (2^{(2n-3/3)} - 2^{(n-9/3)} - 1) > 0. \end{aligned} \quad (107)$$

If $n \geq 12$, let $2^{(n-9/3)} = x \geq 2$, then $2^{(2n-3/3)} - 2^{(n-9/3)} - 1 = 32x^2 - x - 1 > 0$. Thus, we get $g_7(n) > g_8(n)$ for $n \geq 12$.

$$\begin{aligned}
g_1(n) - g_5(n) &= 3 \cdot 2^{n-6} + 13 \cdot 2^{(2n-19/3)} + 2^{(n-8/3)} \\
&\quad - 23 \cdot 2^{(3n-34/4)} - 3 \cdot 2^{(n-10/2)} - 2^{(n-14/4)} \\
&= 2^{(3n-34/4)} (3 \cdot 2^{(n+10/4)} - 23) \\
&\quad + 2^{(n-10/2)} (13 \cdot 2^{(n-8/6)} - 3) \\
&\quad + 2^{(n-14/4)} (2^{(n+10/12)} - 3).
\end{aligned} \tag{108}$$

If $n \geq 14$, then $3 \cdot 2^{(n+10/4)} - 23 > 0$, $13 \cdot 2^{(n-8/6)} - 3 > 0$, and $2^{(n+10/12)} - 3 > 0$. Thus, we get $g_1(n) > g_5(n)$ for $n \geq 14$.

$$\begin{aligned}
g_5(n) - g_6(n) &= 2^{n-6} + 23 \cdot 2^{(3n-34/4)} + 3 \cdot 2^{(n-10/2)} \\
&\quad + 2^{(n-14/4)} \\
&\quad - 9 \cdot 2^{(4n-56/5)} - 2^{(3n-27/5)} \\
&> 2^{(4n-56/5)} (2^{(n+26/5)} - 9) \\
&\quad + 2^{(3n-27/5)} (23 \cdot 2^{(3n-62/20)} - 1).
\end{aligned} \tag{109}$$

If $n \geq 21$, then $2^{(n+26/5)} - 9 > 0$ and $23 \cdot 2^{(3n-62/20)} - 1 > 0$. Thus, we get $g_5(n) > g_6(n)$ for $n \geq 21$.

$$\begin{aligned}
g_8(n) - g_6(n) &= 2^{n-5} + 31 \cdot 2^{(2n-24/3)} + 3 \cdot 2^{(n-12/3)} \\
&\quad - 9 \cdot 2^{(4n-56/5)} - 2^{(3n-27/5)} \\
&> 2^{(4n-56/5)} (2^{(n+31/5)} - 9) \\
&\quad + 2^{(3n-27/5)} (31 \cdot 2^{(n-39/15)} - 1).
\end{aligned} \tag{110}$$

If $n \geq 14$, then $2^{(n+31/5)} - 9 > 0$ and $31 \cdot 2^{(n-39/15)} - 1 > 0$. Thus, we get $g_8(n) > g_6(n)$ for $n \geq 14$.

By above calculation comparison, we get $g_6(n) < g_i(n)$, where $i = 1, 2, 3, 4, 5, 7, 8, 9$, for $n \geq 29$. A direct computation yields $i(C_8) = 18$, $i(C_9) = 29$. Thus, the graph H_6^* has the minimum Merrifield-Simmons index among all graphs in $\mathcal{V}_n^4$ if $n \geq 29$.

5. Summary and Conclusions

In this paper, we investigate extremal properties of the Merrifield-Simmons 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. Special analytical results for the Merrifield-Simmons index contribute to a better understanding of molecular topology when using this measure.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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