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Largest Hosoya Index and Smallest Merrifield–Simmons Index in Tricyclic Graphs*

Yan Liu, Wei Zhuang, Zefang Liang

Department of Mathematics, South China Normal University, Guangzhou, 510631, P.R. China

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Abstract A tricyclic graph is a connected simple graph with n vertices and $n+2$ edges. A bicyclic graph is a connected simple graph with n vertices and $n+1$ edges. Hosoya index of a graph is the total number of its matchings. Merrifield–Simmons index of a graph is the total number of its independent sets. In this paper, we point out errors about the largest Hosoya index of bicyclic graphs in the paper published in *Computers and Mathematics with Applications* in 2008, and then the tricyclic graphs with the largest Hosoya index and with the smallest Merrifield–Simmons index are characterized, respectively. Thus we find that the tricyclic graph that maximizes the Hosoya index and the one that minimizes the Merrifield–Simmons index are completely different.

1. Introduction and Preliminaries

The Hosoya index of a graph G is defined as the total number of matchings (including the empty set) and is denoted by $z(G)$. The Merrifield–Simmons index of G is defined as the total number of independent sets (including the empty set) and is denoted by $\sigma(G)$. A simple connected graph with n vertices and $n+2$ edges is said to be a tricyclic graph.

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Correspondence should be addressed to Yan Liu (e-mail: liuyan@scnu.edu.cn)

The Hosoya index and the Merrifield–Simmons index are typical examples of graph invariants used in mathematical chemistry for quantifying relevant details of molecular structure (see [1,2]). In recent years, a lot of work has been done on the extremal problem for these two indices (see [3–10]). The two indices do not only have very similar definitions, they are also quite related in other respects [8]: for many graph classes, the graph that minimizes (maximizes) the Hosoya index is also the one that maximizes (minimizes) the Merrifield–Simmons index and vice versa. How about the two indices in tricyclic graphs? [6] and [7] show that the extremal graph with the largest Merrifield–Simmos index is the one with the smallest Hosoya index among all tricyclic graphs. In this paper, we characterize the tricyclic graph with the largest Hosoya index and the one with the smallest Merrifield–Simmons index, respectively. Thus we find that the graph that maximizes the Hosoya index and the one that minimizes the Merrifield–Simmons index are completely different. To prove the results, we need to know the largest Hosoya index of bicyclic graphs. However, we find that the result about the largest Hosoya index of bicyclic graphs reported by Deng [9] is wrong and we give a new proof in this paper.

Let G be a simple graph. For any $v \in V(G)$, let $N_G(v) = \{u|uv \in E(G)\}$, $N_G[v] = N_G(v) \cup \{v\}$ and $d_G(v) = |N_G(v)|$ is said to be the degree of v in G. A path P of G is said to be a pending path if either P has only one edge or all internal vertices of P have degree two in G, and a cycle C of G is said to be a pending cycle if all vertices of C have degree two in G except one vertex. If components of G are $G_1, \ldots, G_t$, then let $G = G_1 \cup \ldots \cup G_t$. P_n and C_n denote the path and the cycle with n vertices, respectively. The Fibonacci number $f(n)$ is the integer such that $f(n) = f(n-1) + f(n-2)$ for $n \geq 2$ with $f(0) = 0$ and $f(1) = 1$.

The following basic results are needed, where (1)–(5) can be found in the references cited [9,10] and (6)–(7) can be obtained by (1)–(4).

Proposition 1.1. (1) Let $G = G_1 \cup \ldots \cup G_t$. Then $z(G) = \prod_{i=1}^{t} z(G_i)$ and $\sigma(G) = \prod_{i=1}^{t} \sigma(G_i)$.
(2) $z(P_n) = f(n+1)$, $\sigma(P_n) = f(n+2)$, and $z(C_n) = \sigma(C_n) = f(n-1) + f(n+1)$.
(3). Let $uv \in E(G)$. Then $z(G) = z(G - \{u, v\}) + z(G - uv)$ and $\sigma(G - uv) > \sigma(G)$.

(4) Let $v \in V(G)$. Then $z(G) = z(G-v) + \sum z(G - \{u,v\})$, over all $u \in N_G(v)$ and $\sigma(G) = \sigma(G-v) + \sigma(G - N_G[v])$.
(5) $f(n) = f(k)f(n-k+1) + f(k-1)f(n-k)$ for any $1 \le k \le n$.
(6) If $s = 3$, then $\sigma(H_1) = f(k+3) + f(k+1)$; $z(H_1) = f(s+k) + f(k)f(s-1)$; $z(H_2) = f(s+k) + f(k)f(s-1) + f(k-1)f(s)$; $z(H_3) = f(s+1)f(t+k+2) + f(s)f(t+1)f(k+1)$, where H_1, H_2 and H_3 are shown in Figure 1.1.
(7) $f(s)f(k) < f(s-1)f(k) + f(s)f(k-1)$ for any $k \ge 2$ and $s \ge 2$.

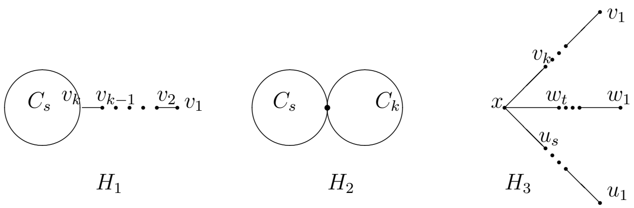

Figure 1.1 Graphs in Proposition 1.1

Now we give three transformations to increase the Hosoya index and decrease the Merrifield–Simmons index as follows.

Lemma 1.1. (Transformation 1 [8]) Let G be a connected graph, T an induced subgraph of G such that T is a tree, T is not a path, T and G only share a cut vertex u and G_1 the graph obtained from G by replacing T with a path P such that P and G also only share u, $|V(P)| = |V(T)|$ and u is an end vertex of P. Then $z(G) < z(G_1)$ and $\sigma(G) > \sigma(G_1)$.

Lemma 1.2. (Transformation 2 [8]) Let $u, v \in V(G)$, $vt_1t_2\cdots t_su$, $uu_1u_2\cdots u_k$ and $vv_1v_2\cdots v_m$ pending paths of G, where $d_G(u_k) = d_G(v_m) = 1$, $s \ge 0$ and $uv \in E(G)$ in the case that $s = 0$, $G_1 = G - \{vv_1\} + \{u_kv_1\}$ and $G_2 = G - \{uu_1\} + \{v_mu_1\}$(see Figure 1.2). Then $z(G) < z(G_1)$ or $z(G) < z(G_2)$ and $\sigma(G) > \sigma(G_1)$ or $\sigma(G) > \sigma(G_2)$.

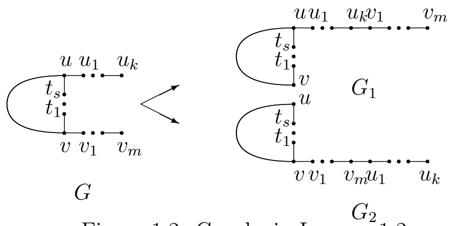

Figure 1.2. Graphs in Lemma 1.2

Lemma 1.3.(Transformation 3)([9]-[10]) Let G and G_1 be the graphs as shown in Figure 1.3, where $0 \leq r \leq t$, $d_G(u_i) = 2$ for any $1 \leq i \leq t$ except $i = r$, $u_r v_{k-1} v_{k-2} \cdots v_1$ be a pending path, $d_G(v_1) = 1$ and $G_1 = G - u_r u_{r+1} + u_{r+1} v_1$. Then $z(G) < z(G_1)$ and $\sigma(G) > \sigma(G_1)$.

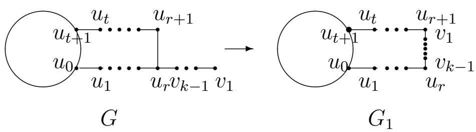

Figure 1.3. Graphs in Lemma 1.3

By Lemma 1.1, Lemma 1.2 and Lemma 1.3, for any bicyclic graph H and any tricyclic graph G, we can repeat Transformation 1, Transformation 2 and Transformation 3 on H and G until get a bicyclic graph H' with no vertices of degree one and a tricyclic graph G' with no vertices of degree one, respectively. Then $z(H) \leq z(H')$, $z(G) \leq z(G')$, $\sigma(G) \geq \sigma(G')$ and the equalities hold if and only if $H \cong H'$ and $G \cong G'$. Let $\mathcal{G}(n, n+1)$ and $\mathcal{G}(n, n+2)$ be the set of the bicyclic graphs with no vertices of degree one and tricyclic graphs with no vertices of degree one, respectively. Then in order to find the largest Hosoya index among all bicyclic and tricyclic graphs and the smallest Merrifield–Simmons index among all tricyclic graphs, we only need to consider the bicyclic graphs in $\mathcal{G}(n, n+1)$ and the tricyclic graphs in $\mathcal{G}(n, n+2)$ in the following.

For convenience, we can divide all graphs G in $\mathcal{G}(n, n+2)$ into following cases by the number of components of G_c, say $w(G_c)$, where G_c is the subgraph induced by all the vertices on a cycle of G. Since $|E(G)| = |V(G)| + 2$, G has three basic cycles, say C_p, C_q and C_l.

Case 1. $w(G_c) = 1$.

We divide into three subcases:

Subcase 1.1. Let $\mathcal{A}(p, q, l, r)$ be the set of $G \in \mathcal{G}(n, n+2)$ in which C_p, C_q and C_l have r common vertices, where $r \geq 1$, as shown in Figure 1.4($\mathcal{A}$).

Subcase 1.2. Let $\mathcal{B}(p, q, l, t, r)$ be the set of $G \in \mathcal{G}(n, n+2)$ in which $r = |V(C_p) \cap V(C_q)| \geq 1$, $t = |V(C_q) \cap V(C_l)| \geq 1$ and $V(C_p) \cap V(C_l) = \emptyset$ as shown in Figure 1.4($\mathcal{B}$).

Subcase 1.3. Let $\mathcal{C}(p, q, l, s, t, r)$ be the set of $G \in \mathcal{G}(n, n+2)$ in which $s = |V(C_p) \cap V(C_q)| \geq 1$, $t = |V(C_q) \cap V(C_l)| \geq 1$, $r = |V(C_p) \cap V(C_l)| \geq 1$, $|V(C_p) \cap V(C_q) \cap V(C_l)| = 1$ and $s + t + r \geq 4$. See Figure 1.4($\mathcal{C}$).

Case 2. $w(G_c) = 2$.

Let $\mathcal{D}(p, q, l, r)$ be the set of $G \in \mathcal{G}(n, n+2)$ in which C_p and C_q have r common vertices, but C_l is disjoint with both C_p and C_q, as shown in Figure 1.4($\mathcal{D}$).

Case 3. $w(G_c) = 3$.

Let $\mathcal{E}(p, q, l)$ be the set of $G \in \mathcal{G}(n, n+2)$ in which C_p, C_q and C_l are disjoint with one another, as shown in Figure 1.4($\mathcal{E}$).

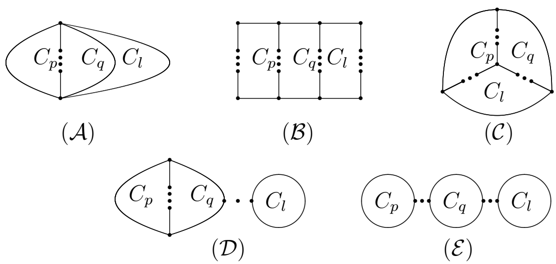

Figure 1.4.

2. Largest Hosoya index in $\mathcal{G}(n, n+1)$

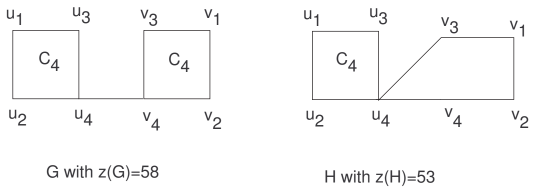

Figure 2.1.

For any $G \in \mathcal{G}(n, n+1)$, G has two basic cycles C_p and C_q. Thus we can divide $\mathcal{G}(n, n+1)$ into two subsets: $\mathcal{G}_1(n, n+1) = \{G \in \mathcal{G}(n, n+1) | \quad V(C_p) \cap V(C_q) \neq \emptyset\}$ and $\mathcal{G}_2(n, n+1) = \mathcal{G}(n, n+1) - \mathcal{G}_1(n, n+1)$. Denote by $\theta(0, 2, n-4)$ the graph in $\mathcal{G}_1(n, n+1)$ consisting of C_4 and C_{n-4} joined by a cut edge (see Figure 2.3).

The result in [9] that the bicyclic graph with largest Hosoya index is $\theta(0, 2, n-4)$ is wrong. We think that the reason resulting this error is that Lemma 3.3 in [9] is wrong (Lemma 3.3[9]: If $G \in \mathcal{G}_2(n, n+1)$ and $H \in \mathcal{G}_1(n, n+1)$ obtained from G by deleting an edge and adding other edge such that two cycle of H share exactly one common vertex, then $z(G) < z(H)$). We give a counterexample (see Figure 2.1) and we will prove that the bicyclic graph with largest Hosoya index is G^{**} (see Figure 2.3).

Lemma 2.1. Let G and H be the graphs as shown in Figure 2.1, where $H = G - v_1v_s + v_1v_4$ and $s \neq 4$. Then $z(G) < z(H)$ if either $k > s$ or $k = s \geq 5$ and $z(G_0) < 2z(G_0 - u)$.

Proof. Let $v_{k+1} = u$. We distinguish the three cases in the following.

Case 1. $k > s = 3$.

Then $G - v_1v_3 = H - v_1v_4$. By Proposition 1.1(1)-(4),

$$\begin{aligned} z(G) - z(H) &= z(G - v_1v_3) + z(G - \{v_1, v_3\}) - z(H - v_1v_4) - z(H - \{v_1, v_4\}) \\ &= z(G - \{v_1, v_2, v_3\}) - 2z(G - \{v_1, v_2, v_3, v_4\}) \\ &= z(G - \{v_1, v_2, v_3, v_4\}) + z(G - \{v_1, v_2, v_3, v_4, v_5\}) \\ &- 2z(G - \{v_1, v_2, v_3, v_4\}) < 0 \ . \end{aligned}$$

Case 2. $k > s \geq 5$.

Then $G - v_1v_s = H - v_1v_4$. By Proposition 1.1(1)-(5),

$$\begin{aligned} z(G) - z(H) &= z(G - \{v_1, v_s\}) - z(H - \{v_1, v_4\}) \\ &= f(s-1)z(G - \{v_1, \cdots, v_s\}) - 2z(H - \{v_1, v_2, v_3, v_4\}) \\ &= f(s-1)z(G - \{v_1, \cdots, v_s\}) \\ &- 2z(H - \{v_1, v_2, v_3, v_4\} - v_sv_{s+1}) - 2z(H - \{v_1, v_2, v_3, v_4, v_s, v_{s+1}\}) \\ &= f(s-1)z(G - \{v_1, \cdots, v_s\}) - 2f(s-3)z(G - \{v_1, \cdots, v_s\}) \\ &- 2f(s-4)z(G - \{v_1, \cdots, v_s, v_{s+1}\}) \\ &= f(s-4)z(G - \{v_1, \cdots, v_s\}) - 2f(s-4)z(G - \{v_1, \cdots, v_s, v_{s+1}\}) \\ &= f(s-4)z(G - \{v_1, \cdots, v_s, v_{s+1}, v_{s+2}\}) \\ &- f(s-4)z(G - \{v_1, \cdots, v_s, v_{s+1}\}) < 0\ . \end{aligned}$$

Case 3. $k = s \geq 5$ and $z(G_0) < 2z(G_0 - u)$.

By Proposition 1.1(1)-(5),

$$\begin{aligned} z(G) - z(H) &= z(G - uv_s) + z(G - \{u, v_s\}) - z(H - uv_s) - z(H - \{u, v_s\}) \\ &= (f(s-1) + f(s+1))z(G_0) + f(s)z(G_0 - u) \\ &- (f(s+1) + f(3)f(s-3))z(G_0) - (f(s) + f(3)f(s-4))z(G_0 - u) \\ &= f(s-4)z(G_0) - 2f(s-4)z(G_0 - u) < 0\ . \end{aligned}$$

Figure 2.2. Graphs in Lemma 2.1

Lemma 2.2.([9]) Let $n \geq 8$. Then for any $G \in \mathcal{G}_1(n, n+1)$, $z(G) \leq z(\theta(0, 2, n-4)) = f(n+1) + f(n-1) + 2f(n-3)$ and the equality holds if and only if $G \cong \theta(0, 2, n-4)$.

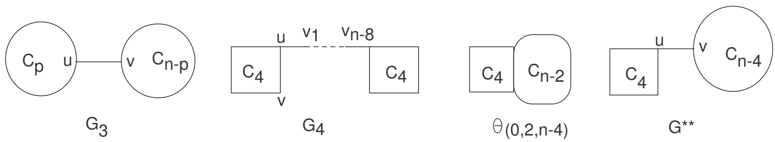

Figure 2.3.

Lemma 2.3. Let $n \geq 8$. Then for any $G \in \mathcal{G}_2(n, n+1)$, $z(G) \leq z(G^{**}) = f(n+1) + 2f(n-3) + 7f(n-5)$ and the equality holds if and only if $G \cong G^{**}$ (see Figure 2.2).

Proof. By Lemma 2.1, it suffices to prove that $z(G_3) < z(G^{**})$ and $z(G_4) < z(G^{**})$, where $G_3 \ncong G^{**}$ and $G_4 \ncong G^{**}$. By Proposition 1.1 (1)-(6),

$$\begin{aligned}
z(G_3) &= z(G_3 - uv) + z(G_3 - \{u,\ v\}) \\
&= [f(p+1) + f(p-1)][f(n-p-1) + f(n-p+1)] + f(p)f(n-p) \\
&= f(n-1) + f(p)f(n-p+1) + f(p-1)f(n-p) + 2f(p-1)f(n-p-1) \\
&+ f(p-1)f(n-p+1) + f(p)f(n-p-1)
\end{aligned}$$

$$\begin{aligned}
z(G^{**}) &= z(G^{**} - uv) + z(G^{**} - \{u,\ v\}) \\
&= 7(f(n-3) + f(n-5)) + 3f(n-4) \\
&= f(n-1) + f(n) + 2f(n-3) + 7f(n-5) \\
&= f(n-1) + f(p)f(n-p+1) + f(p-1)f(n-p) \\
&+ 2f(p-1)f(n-p-1) + 2f(p-2)f(n-p-2) \\
&+ 7f(p-2)f(n-p-2) + 7f(p-3)f(n-p-3)
\end{aligned}$$

$$\begin{aligned} z(G^{**}) - z(G_3) &= 9f(p-2)f(n-p-2) + 7f(p-3)f(n-p-3) \\ &- f(p)f(n-p-1) - f(p-1)f(n-p+1) \\ &= 4f(p-4)f(n-p-4) > 0 \end{aligned}$$

$$\begin{aligned} z(G_4) &= z(G_4 - uv) + z(G_4 - \{u,\ v\}) \\ &= f(n+1) + 2f(n-3) + 2(f(n-3) + 2f(n-7)) \\ z(G^{**}) - z(G_4) &= 7f(n-5) - 2f(n-3) - 4f(n-7) = f(n-8) > 0\ . \end{aligned}$$

Theorem 2.4. If $n \leq 7$, then $\theta(0, 2, n-4)$ is the graph with the largest Hosoya index in $\mathcal{G}(n, n+1)$; If $n = 9$, then $\theta(0, 2, n-4)$ and G^{**} are the graphs with the largest Hosoya index in $\mathcal{G}(n, n+1)$; If $n = 8$ or $n \geq 10$, then G^{**} is the unique graph with the largest Hosoya index in $\mathcal{G}(n, n+1)$.

Proof. When $n \leq 7$, it is easy to check that $\theta(0, 2, n-4)$ is the graph with the largest Hosoya index in $\mathcal{G}(n, n+1)$. When $n = 8$, $z(G^{**}) = 58$ and $z(\theta(0, 2, n-4)) = 57$. When $n = 9$, $z(G^{**}) = z(\theta(0, 2, n-4)) = 92$. When $n \geq 10$,
$z(G^{**}) - z(\theta(0, 2, n-4)) = f(n+1) + 2f(n-3) + 7f(n-5) - f(n+1) - f(n-1) - 2f(n-3)$
$= 7f(n-5) - f(n-1) = 2f(n-5) - 3f(n-6) = f(n-9) > 0.$

By Lemma 2.2 and Lemma 2.3, the statement holds.

3. Largest Hosoya index in $\mathcal{G}(n, n+2)$

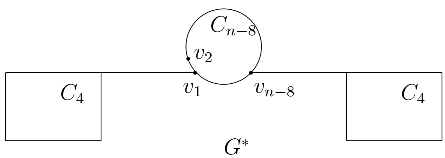

Figure 3.1. Tricycle graph with the largest Hosoya index

In this section, we will prove the following theorem.

Theorem 3.1. Let $G \in \mathcal{G}(n, n+2)$ and $n \geq 15$. Then $z(G) \leq 33f(n-6) + 25f(n-7) + 49f(n-9)$ and the equality holds if and only if $G \cong G^*$.

We distinguish the following five cases to prove Theorem 3.1.

3.1. Graph with the largest Hosoya index in $\mathcal{E}(p, q, l)(n \geq 14)$

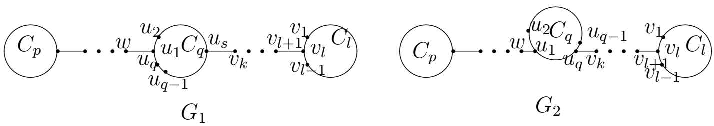

Figure 3.1.1 Graphs in Lemma 3.1.1

Lemma 3.1.1. Let G_1 and G_2 be the graph as shown in Figure 3.1.1, where $G_2 = G_1 - u_s v_k + u_q v_k$ and $3 \leq s \leq q-1$ or $s = 1$. Then $z(G_1) < z(G_2)$.

Proof. Since $G_1 - u_s v_k = G_2 - u_q v_k$ and by Proposition 1.1 (1)-(4), $z(G_1) - z(G_2) = z(G_1 - \{u_s,\ v_k\}) - z(G_2 - \{u_q,\ v_k\})$. Suppose that $3 \leq s \leq q-1$. Then by Lemma 1.1, $z(G_1 - \{u_s,\ v_k\}) < z(G_2 - \{u_q,\ v_k\})$. If $s = 1$, then $G_1 - \{u_s, v_k\} \cong G_2 - \{u_q, v_k\} - wu_1$. So, $z(G_1 - \{u_s,\ v_k\}) < z(G_2 - \{u_q,\ v_k\})$. Hence $z(G_1) < z(G_2)$.

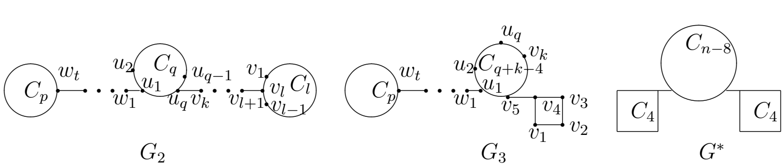

Figure 3.1.2 Graphs in Lemma 3.1.2

Lemma 3.1.2. Let G_2, G_3 and G^* be the graphs as shown in Figure 3.1.2, $G_2 \not\cong G_3$ and $G_3 \not\cong G^*$. Then $z(G_2) < z(G_3) < z(G^*)$.

Proof. Without loss of generality, we can assume that $q + k \geq 9$ since $n \geq 14$. In fact, if $v_{k+1} = u_q, \ldots, v_{q+k} = u_1$, then $G_3 = G_2 - v_1v_l + v_1v_4 - u_1u_q + u_1v_5$.

$$z(G_2) - z(G_3) = z(G_2 - w_1u_1) + z(G_2 - \{w_1,\ u_1\}) - [z(G_3 - w_1u_1) + z(G_3 - \{w_1,\ u_1\})]$$
$$= [z(G_2 - w_1u_1) - z(G_3 - w_1u_1)] + [z(G_2 - \{w_1,\ u_1\}) - z(G_3 - \{w_1,\ u_1\})]$$

By Theorem 2.4, $z(G_2 - w_1u_1) - z(G_3 - w_1u_1) < 0$. By Lemma 2.1, $z(G_2 - \{w_1,\ u_1\}) - z(G_3 - \{w_1,\ u_1\}) \leq 0$. So, $z(G_2) < z(G_3)$. By the above method, we can obtain that $z(G_3) < z(G^*)$.

In the following, we consider the graphs G_4 as shown in Figure 3.1.3. Then either one in $\{s, t, r\}$ is at least 2 or $s = t = r = 1$ and one in $\{p, q, l\}$ is at least 5 since $n \geq 14$. Without loss of generality, we can assume that $r \geq 2$ or $s = t = r = 1$ and $l \geq 5$.

Lemma 3.1.3. Let G_4 and G_5 be the graphs as shown in Figure 3.1.3, where $l \neq 4$. Then $z(G_4) < z(G_5)$.

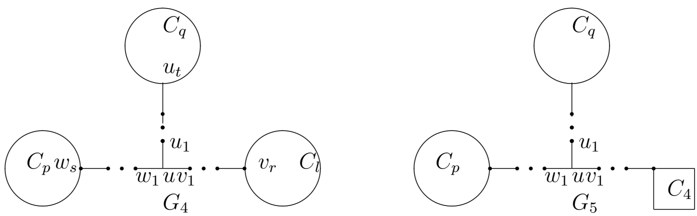

Figure 3.1.3. Graphs in Lemma 3.1.3

Proof. When $r \geq 2$, $z(G_4) < z(G_5)$ by Lemma 2.1. Suppose that $s = t = r = 1$ and $l \geq 5$. Let G_0 be the component of $G_4 - v_1u$ containing C_p and C_q. By Lemma 2.1, it suffices to prove that $z(G_0) < 2z(G_0 - u)$. By Proposition 1.1 (4) and (7),

$$\begin{aligned} z(G_0) - 2z(G_0 - u) &= f(p)(f(q+1) + f(q-1)) + f(q)(f(p+1) + f(p-1)) \\ &- (f(p+1) + f(p-1))(f(q+1) + f(q-1)) \end{aligned}$$

$$= f(q)(f(p+1)+f(p-1))-2f(p-1)(f(q+1)+f(q-1))$$
$$= f(q)(f(p)+2f(p-1))-2f(p-1)(f(q)+2f(q-1))$$
$$= f(q)f(p)-4f(p-1)f(q-1)<0\ .$$

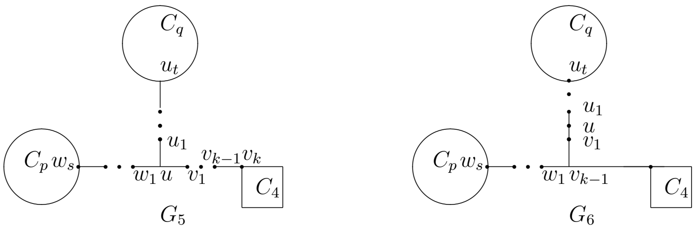

Figure 3.1.4. Graphs in Lemma 3.1.4

Lemma 3.1.4. Let G_5 and G_6 be the graphs as shown in Figure 3.1.4, where $k \geq 2$ and $G_6 = G_5 - w_1u + w_1v_{k-1}$. Then $z(G_5) < z(G_6)$.

Proof. Let G' be the component of $G_5 - w_1$ containing C_p. By Proposition 1.1,

$$\begin{aligned}
z(G_5)-z(G_6) &= z(G_5-\{w_1,u\})-z(G_6-\{w_1,v_{k-1}\})\\
&= z(G')[(f(q+t)+f(q-1)f(t))(f(k+4)\\
&+ f(3)f(k))-7(f(q+t+k-1)+f(q-1)f(k+t-1))]\\
&= z(G')[(f(q+t)+f(q-1)f(t))(7f(k)+3f(k-1))\\
&- 7(f(q+t)f(k)+f(q+t-1)f(k-1)\\
&+ f(q-1)(f(t)f(k)+f(t-1)f(k-1)))]\\
&= z(G')f(k-1)[3(f(q+t)+f(q-1)f(t))\\
&- 7(f(q+t-1)+f(q-1)f(t-1))]<0\ .
\end{aligned}$$

Lemma 3.1.5. Let G_6, G_7 and G^* be the distinct graphs as shown in Figure 3.1.4 and Figure 3.1.5. Then $z(G_6) < z(G_7) < z(G^*) = 33f(n-6)+25f(n-7)+49f(n-9)$.

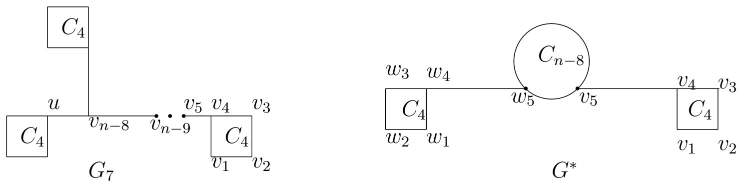

Figure 3.1.5. Graphs in Lemma 3.1.5

Proof. By Lemma 3.1.3 and Lemma 3.1.4, $z(G_6) < z(G_7)$. By Proposition 1.1,

$$\begin{aligned} z(G_7) &= z(G_7 - v_{n-8}\,u) + z(G_7 - \{v_{n-8},\ u\}) \\ &= 49(f(n-7) + 2f(n-11)) + 42(f(n-8) + 2f(n-12)) \\ &= 42f(n-6) + 7f(n-7) + 14f(n-9) + 70f(n-10)\ . \end{aligned}$$

$$\begin{aligned} z(G^*) &= z(G^* - w_4\,w_5) + z(G^* - \{w_4,\ w_5\}) \\ &= 7[7f(n-7) + 7f(n-9) + 3f(n-8)] + 3f(n-4) + 6f(n-8) \\ &= 33f(n-6) + 25f(n-7) + 49f(n-9)\ . \end{aligned}$$

Then

$$z(G_7) - z(G^*) = 9f(n-6) + 70f(n-10) - 18f(n-7) - 35f(n-9) < 0\ .$$

3.2. Graphs in $\mathcal{D}(p,q,l,r)$ with $n \geq 15$

The graphs in $\mathcal{D}(p,q,l,r)$ are shown as G_8 and G_8' in Figure 3.2.1. We prove that there exists a graph $G \in \mathcal{E}(p,q,l,r)$ such that $z(G_8) \leq z(G)$ and $z(G_8') \leq z(G)$.

Lemma 3.2.1. Let G_8, G_8' and G_9 be the graphs as shown in Figure 3.2.1, where $2 \leq i \leq k-1$. Then $z(G_8) < z(G_9)$ and $z(G_8') < z(G_9)$.

Proof. By Lemma 1.2, we can assume that $G_9 = G_8' - w_1y_i + w_1y_1$ such that $z(G_8' - \{w_1, y_i\}) < z(G_9 - \{w_1, y_1\})$ without loss of generality. Then $z(G_8') < z(G_9)$.

Note that $G_9 = G_8 - x_1w_1 + w_1y_1$. Let G' be the component of $G_8 - x_1w_1$ containing C_l and $m = z(G' - w_1)$. Then G' is also the component of $G_9 - y_1w_1$. Let $H_8 = G_8 - V(G') - x_1$

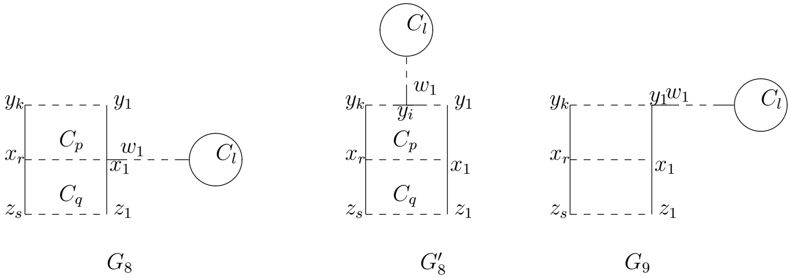

Figure 3.2.1. Graphs in Lemma 3.2.1

and $H_9 = G_9 - V(G') - y_1$. By Proposition 1.1,

$$z(G_8) - z(G_9) = z(G_8 - \{x_1, w_1\}) - z(G_9 - \{y_1, w_1\}) = m(z(H_8) - z(H_9)) \ .$$

Case 1. $r = 1$.

Then $x_1 = x_r$ and x_1 is a cut vertex of G_8 and G_9. Clearly, $H_8 \cong H_9 - \{x_1z_1, x_1z_s\}$. Then $z(H_8) - z(H_9) < 0$.

Case 2. $r > 1$.

Then H_8 is a tree. By Lemma 1.1, $z(H_8) \leq z(P_{k+s+r-1})$. Clearly, $P_{k+s+r-1}$ is isomorphic to $H_9 - x_rz_s$. Then $z(P_{k+s+r-1}) < z(H_9)$. Hence $z(H_8) - z(H_9) < 0$.

Figure 3.2.2. Graphs in Lemma 3.2.2

Lemma 3.2.2. Let G_9 and G_{10} be the graphs as shown in Figure 3.2.2, where $r \neq 2$. Then $z(G_9) < z(G_{10})$.

Proof. Note that $G_{10} = G_9 - y_k x_r + y_k x_2$ if $r \geq 3$ and $G_{10} = G_9 - y_k x_r + y_k z_s$ if $r = 1$.

Case 1. $r = 1$.

Then $x_1 = x_r$ and x_1 is a cut vertex of G_9. Clearly, $G_9 - \{y_k, x_r\} \cong G_{10} - \{y_k, z_s\} - y_1 x_1$. Then $z(G_9) < z(G_{10})$.

Case 2. $r \geq 3$.

$$z(G_9) - z(G_{10}) = z(G_9 - \{y_k,\ x_r\}) - z(G_{10} - \{y_k,\ x_2\}) < 0 \text{ (By Lemma 1.1).}$$

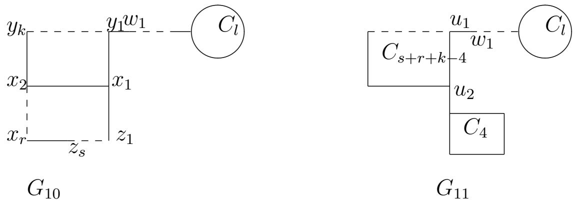

Figure 3.2.3. Graphs in Lemma 3.2.3

Lemma 3.2.3. Let G_{10} and G_{11} be the graphs as shown in Figure 3.2.3, and $s+r+k \geq 8$. Then $z(G_{10}) < z(G_{11})$.

Proof. By Theorem 2.4, $z(G_{10} - y_1 w_1) < z(G_{11} - u_1 w_1)$.

Case 1. $k \geq 2$.

By Lemma 2.1, $z(G_{10} - \{y_1,\ w_1\}) < z(G_{11} - \{u_1,\ w_1\})$. Then $z(G_{10}) < z(G_{11})$.

Case 2. $k = 1$.

Let G' be the component of $G_{10} - y_1 w_1$ containing C_l, $m = z(G')$, $m' = z(G' - w_1)$ and $t = s + r + k$. Then by Proposition 1.1 and Lemma 2.3,

$$z(G_{10}) - z(G_{11}) = z(G_{10} - y_1 w_1) - z(G_{11} - u_1 w_1) + z(G_{10} - \{y_1, w_1\}) - z(G_{11} - \{u_1, w_1\})$$
$$= m(f(t+1) + f(t-1) + f(t-2) - f(t+1) - 2f(t-3) - 7f(t-5))$$
$$+m'(f(t) + f(t-2) - f(t) - 2f(t-4)) = -3mf(t-7) + m'f(t-5) < 0.$$

When $s + r + k \leq 7$, we have the following lemma.

Lemma 3.2.4. Let G_{10}, G_{12} and G_{13} be graphs as shown in Figure 3.2.4. Then $z(G_{10}) < z(G^{*})$.

Proof. By Lemma 2.1, $z(G_{10}) \le z(G_{12})$ if $s \ge 2$. When $s = 1$, $G_{10} = G_{13}$. So it suffices to prove that $z(G_{12}) < z(G^{*})$ and $z(G_{13}) < z(G^{*})$, which can be checked easily, and is therefore omitted.

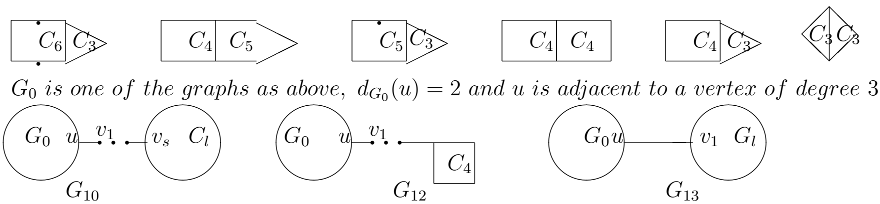

Figure 3.2.4. Graphs in Lemma 3.2.4

3.3. Graph with the largest Hosoya index in $\mathcal{A}(p, q, l, r)$ with $n \ge 15$

The graphs in $\mathcal{A}(p, q, l, r)$ are shown as G_{14} in Figure 3.3.1. We prove that there exists a graph $G \in \mathcal{D}(p, q, l, r)$ such that $z(G_{14}) \le z(G)$. Without loss of generality, suppose that $t \ge s \ge k \ge r - 2$ and x_1 is a cut vertex in the case that $r = 1$. Since $n \ge 15$, we have $t \ge 4$.

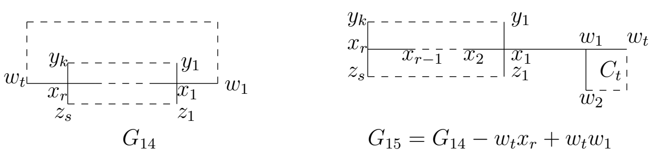

Figure 3.3.1. Graphs in Lemma 3.3.1

Lemma 3.3.1. Let G_{14} and G_{15} be the graphs as shown in Figure 3.3.1. Then $z(G_{14}) < z(G_{15})$.

Proof. Case 1. $r = 1$.

By Proposition 1.1 (3)-(6), we have the following.

$$
\begin{aligned}
& z(G_{14}) - z(G_{15}) = z(G_{14} - \{w_t,\ x_r\}) - z(G_{15} - \{w_t, w_1\}) \\
= \ & f(t)f(s+1)f(k+1) - f(t-1)(f(s+k+2) + f(s)f(k+1) + f(s+1)f(k)) \\
= \ & f(t)f(s+1)f(k+1) - f(t-1)(f(s+1)f(k+2) + 2f(s)f(k+1) + f(s+1)f(k)) \\
= \ & f(t-2)f(s+1)f(k+1) - f(t-1)(2f(s)f(k+1) + 2f(s+1)f(k)) < 0 \ .
\end{aligned}
$$

Case 2. $r \geq 2$.

It is easy to check that $G_{14} - \{w_t, x_r, x_1, w_1\} \cong G_{15} - \{w_t,\ w_1, x_r, y_k\} - \{x_1 x_2, x_1 z_1\}$. Since $G_{14} - \{w_t, x_r, w_1\} = G_{15} - \{w_t, w_1, x_r\}$ and by Proposition 1.2(3)-(7),

$$
\begin{aligned}
& z(G_{14}) - z(G_{15}) = z(G_{14} - \{w_t, x_r\}) - z(G_{15} - \{w_t, w_1\}) \\
= \ & z(G_{14} - \{w_t, x_r, w_1, x_1\}) + z(G_{14} - \{w_t, x_r, w_1, w_2\}) \\
- \ & z(G_{15} - \{w_t, w_1, x_r, y_k\}) - z(G_{15} - \{w_t, w_1, x_r, z_s\}) - z(G_{15} - \{w_t, w_1, x_r, x_{r-1}\}) \\
\leq \ & z(G_{14} - \{w_t, x_r, w_1, w_2\}) - z(G_{15} - \{w_t, w_1, x_r, z_s\}) - z(G_{15} - \{w_t, w_1, x_r, x_{r-1}\}) \\
= \ & f(t-2)(f(s+1)f(k+r) + f(s)f(k+1)f(r-1)) \\
- \ & f(t-1)[f(s)f(k+r) + f(s-1)f(k+1)f(r-1) \\
+ \ & f(s+1)f(k+r-1) + f(s)f(k+1)f(r-2)] \\
< \ & f(t-2)[f(s+1)f(k+r) - (f(s)f(k+r) + f(s+1)f(k+r-1)) \\
+ \ & f(k+1)(f(s)f(r-1) - (f(s-1)f(r-1) + f(s)f(r-2)))] < 0 \text{ if } r \geq 3 \ .
\end{aligned}
$$

If $r = 2$, then

$$
\begin{aligned}
z(G_{14}) - z(G_{15}) \ &< \ f(t-2)[f(s+1)f(k+2) - f(s)f(k+2) \\
&- \ f(s+1)f(k+1) + f(k+1)f(s-2) \\
&= \ f(t-2)[f(s-1)f(k+2) - 2f(s-1)f(k+1)] < 0 \ .
\end{aligned}
$$

3.4. Graph with the largest Hosoya index in $\mathcal{B}(p, q, l, t, r)$ with $n \geq 15$

The graphs in $\mathcal{B}(p, q, l, t, r)$ are shown as G_{16} in Figure 3.4.1. Then $u_r \neq v_t$, $u_1 \neq v_1$, $t \geq 1$ and $r \geq 1$.

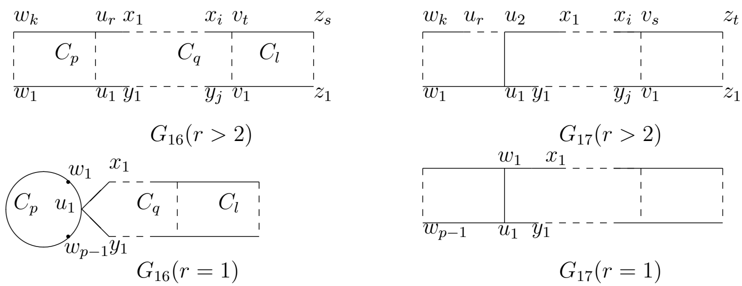

Figure 3.4.1. Graphs in Lemma 3.4.1

Lemma 3.4.1. Let G_{16} and G_{17} be the graphs as shown in Figure 3.4.1. Then $z(G_{16}) < z(G_{17})$.

Proof. Case 1. $r = 1$.

Then u_1 is a cut vertex and $G_{17} = G_{16} - x_1u_1 + x_1w_1$. Note that $G_{16} - \{x_1, u_1\} \cong G_{17} - \{x_1, w_1\} - u_1y_1$. Then we have:

$$z(G_{16}) - z(G_{17}) = z(G_{16} - \{u_1,\ x_1\}) - z(G_{17} - \{w_1,\ x_1\}) < 0\ .$$

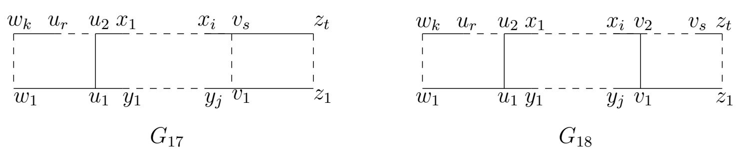

Figure 3.4.2. Graphs in Lemma 3.4.2

Case 2. $r \geq 2$.

Note that $G_{17} = G_{16} - x_1u_r + x_1u_2$. By Lemma 1.1,

$$z(G_{16} - \{x_1, u_r\}) < z(G_{17} - \{x_1, u_2\})$$

Then $z(G_{16}) - z(G_{17}) < 0$.

By Lemma 3.4.1, we obtain the following:

Lemma 3.4.2. Let G_{17} and G_{18} be the graphs as shown in Figure 3.4.2. Then $z(G_{17}) < z(G_{18})$.

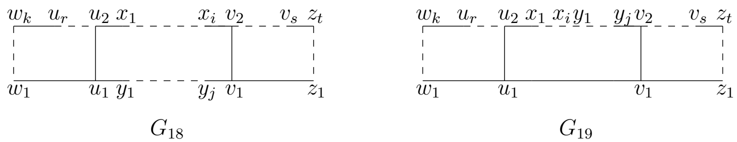

Figure 3.4.3. Graphs in Lemma 3.4.3

Lemma 3.4.3. Let G_{18} and G_{19} be the graphs as shown in Figure 3.4.3. Then $z(G_{18}) < z(G_{19})$.

Proof. Clearly, $G_{18} - v_2v_1 \cong G_{19} - v_2v_1$. Without loss of generality, by Lemma 1.2, we can assume that $z(G_{18} - \{v_2,\ v_1\}) < z(G_{19} - \{v_2,\ v_1\})$. Then $z(G_{18}) < z(G_{19})$.

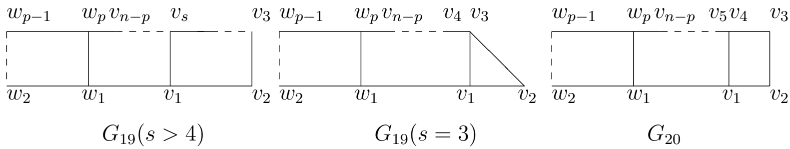

Figure 3.4.4. Graphs in Lemma 3.4.4

Lemma 3.4.4. Let G_{19} and G_{20} be the graphs as shown in Figure 3.4.4. Then $z(G_{19}) < z(G_{20})$.

Proof. **Case 1.** $s > 4$.

Since $G_{20} = G_{19} - v_sv_1 + v_4v_1$, we have the following:

$$\begin{aligned} & z(G_{19}) - z(G_{20}) \\ = \ & z(G_{19} - \{v_s,\ v_1\}) - z(G_{20} - \{v_4,\ v_1\}) \\ = \ & (f(n-s+1) + f(p-1)f(n-p-s+1))f(s-1) - 2(f(n-3) \end{aligned}$$

$$
\begin{aligned}
&+ \quad f(p-1)f(n-p-3)) \\
&= \quad (f(n-s-2)+2f(n-s-1)+f(p-1)f(n-p-s+1))f(s-1) \\
&- \quad 2(f(s-1)f(n-s-1)+f(s-2)f(n-s-2)+f(p-1)f(n-p-3)) \\
&= \quad (f(n-s-2)+f(p-1)f(n-p-s+1))f(s-1) \\
&- \quad 2(f(s-2)f(n-s-2)+f(p-1)f(n-p-3)) \\
&< \quad f(p-1)f(n-p-s+1)f(s-1)-2f(p-1)f(n-p-3) \\
&= \quad f(p-1)f(n-p-s+1)f(s-1)-2f(p-1)(f(s-1)f(n-p-s-1) \\
&+ \quad f(s-2)f(n-p-s-2)) \\
&= \quad f(p-1)f(n-p-s-2)f(s-1)-2f(p-1)f(s-2)f(n-p-s-2)<0\ .
\end{aligned}
$$

Case 2. $s=3$.

Without loss of generality, we can assume that $p \le 4$. (Otherwise, $p>4$, which is the condition in Case 1.) Then $n-p \ge 11$. Clearly, $G_{19}-v_3v_1 \cong G_{20}-v_4v_1$ and $G_{19}-\{v_1,v_2,v_3,v_4\} \cong G_{20}-\{v_1,v_2,v_3,v_4\}$. $z(G_{19}-\{v_3,v_1\})=z(G_{19}-\{v_3,v_1,v_2\})=z(G_{19}-\{v_1,v_2,v_3,v_4\})+z(G_{19}-\{v_1,v_2,v_3,v_4,v_5\})$. $z(G_{20}-\{v_4,v_1\})=2z(G_{20}-\{v_1,v_2,v_3,v_4\})$. Then $z(G_{19})<z(G_{20})$.

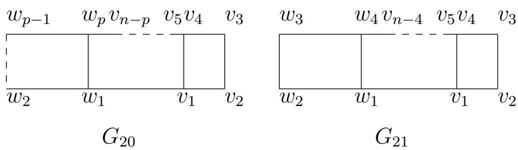

Figure 3.4.5. Graphs in Lemma 3.4.5

Lemma 3.4.5. Let G_{21} be the graph as shown in Figure 3.4.5. Then for any $G \in \mathcal{B}(p,q,l,t,r)$, $z(G) \le z(G_{21})$ and $z(G_{21})<z(G^*)$.

Proof. By Lemma 3.4.1-Lemma 3.4.4, $z(G) \le z(G_{20}) \le z(G_{21})$. By Proposition 1.1 (4) on v_1, it is easy to check that $z(G_{21})=41f(n-6)+30f(n-7)$, so $z(G^*)=33f(n-6)+25f(n-7)+49f(n-9)>z(G_{21})$.

3.5. Graph with the largest Hosoya index in $\mathcal{C}(p,q,l,s,t,r)$ with $n \geq 15$

The graphs in $\mathcal{C}(p,q,l,s,t,r)$ are shown as G_{22} in Figure 3.5.1, where $u = x_1 = y_1 = z_1$. Since $s+t+r \geq 4$, we can assume that $s \geq 2$.

Figure 3.5.1. Graphs in Lemma 3.5.1

Lemma 3.5.1. Let G_{22} and G_{23} be the graphs as shown in Figure 3.5.1, where $s \geq 3$. Then $z(G_{22}) < z(G_{23})$.

Proof. Since $G_{23} = G_{22} - u_1x_s + u_1x_2$, $z(G_{22} - u_1x_s) = z(G_{23} - u_1x_1)$. Without loss of generality, by Lemma 1.2, we can assume that $z(G_{22} - \{u_1,\ x_s\}) < z(G_{23} - \{u_1,\ x_1\})$. Then $z(G_{22}) < z(G_{23})$.

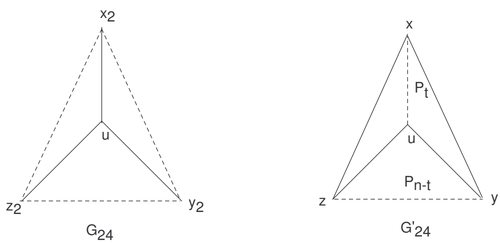

Figure 3.5.2.

Lemma 3.5.2. Let G_{23} be the graph as shown in Figure 3.5.1, where $t \geq r \geq 2$, G_{24} and G'_{24} be the graphs as shown in Figure 3.5.2. Then $z(G_{23}) < z(G^*)$.

Proof. By Lemma 1.2 and the same method as the proof of Lemma 3.5.1, either $z(G_{23}) \leq z(G_{24})$ or $z(G_{23}) \leq z(G'_{24})$, where $ux_2, uy_2, uz_2 \in E(G_{24})$ and $uy, uz, xy, xz \in E(G'_{24})$. By

Proposition 1.1 (4) on u,

$$\begin{aligned} z(G_{24}) &= f(n)+f(n-2)+3f(n-1) = 42f(n-6)+26f(n-7) < z(G^*)\ . \\ z(G'_{24}) &= f(n)+3f(n-1)+f(n-t)f(t) \\ &= 37f(n-6)+23f(n-7)+f(n-t)f(t)\ . \\ z(G'_{24})-z(G^*) &= f(n-t)f(t)-35f(n-9)-6f(n-11) \\ &< f(n-t)f(t)-f(n-2)-f(n-5) \\ &= f(n-t)f(t)-f(n-t)f(t-1)-f(n-t-1)f(t-2) \\ &- f(n-5) = f(n-t-2)f(t-2)-f(n-5) < 0\ . \end{aligned}$$

When $t = r = 1$, $G_{23} = G_{25}$. When $t = 2$ and $r = 1$, $G_{23} = G_{26}$. When $r \geq 3$ and $t = 1$, we can obtained that $z(G_{23}) < z(G_{26})$ by the same method as in the proof of Lemma 3.5.1.

Lemma 3.5.3. Let G_{25} and G_{26} be the graphs as shown in Figure 3.5.3. Then $z(G_{25}) < z(G_{26})$.

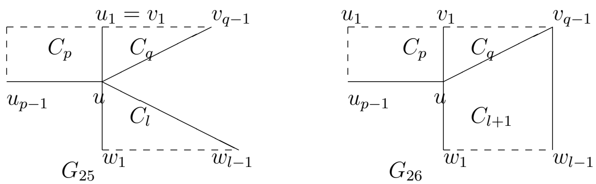

Figure 3.5.3. Graphs in Lemma 3.5.3

Proof. Note that $G_{26} = G_{25} - w_{l-1}u + w_{l-1}v_{q-1}$ and $G_{25} - \{w_{l-1},\ u\} \cong G_{26} - \{w_{l-1},\ v_{q-1}\} - \{uw_1, uv_1\}$. Then $z(G_{25}) - z(G_{26}) = z(G_{25} - \{w_{l-1},\ u\}) - z(G_{26} - \{w_{l-1},\ v_{q-1}\}) < 0$.

Lemma 3.5.4. Let G_{26}, G_{27} and G_{28} be the graphs as shown in Figure 3.5.4 and $q+r \geq 7$ without loss of generality. Then $z(G_{26}) \leq z(G_{28}) < z(G^*)$.

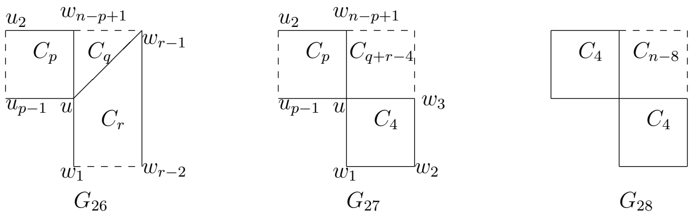

Figure 3.5.4. Graphs in Lemma 3.5.4

Proof. Suppose that $r \neq 4$. Since $G_{27} = G_{26} - uw_{r-1} + uw_3$,

$$\begin{aligned} z(G_{26}) - z(G_{27}) &= z(G_{26} - \{w_{r-1},\ u\}) - z(G_{27} - \{w_3,\ u\}) \\ &= f(r-1)f(n-r+1) - 2f(n-3) \\ &= f(r-1)f(n-r+1) - 2f(r-1)f(n-r-1) \\ &- 2f(r-2)f(n-r-2) \\ &= f(r-1)f(n-r-2) - 2f(r-2)f(n-r-2) \leq 0\ . \end{aligned}$$

Similarly, we have $z(G_{27}) \leq z(G_{28})$. By Proposition 1.1 (2)-(6),

$$\begin{aligned} z(G_{28}) &= 4f(n-3) + f(n+1) + f(n-1) \\ &= 33f(n-6) + 25f(n-7) + 26f(n-9) + 17f(n-10) < z(G^*)\ . \end{aligned}$$

4. Smallest Merrifield–Simmons index in $\mathcal{G}(n, n+2)$

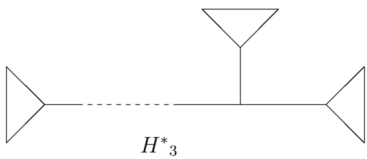

Figure 4.1. Graph with the smallest Merrifield–Simmons index in $\mathcal{G}(n, n+2)$

In this section, we will prove the following theorem.

Theorem 4.1. Let $G \in \mathcal{G}(n, n+2)$ and $n \geq 11$. Then $\sigma(G) \geq 57f(n-8) + 34f(n-9)$ and the equality holds if and only if $G \cong H_3^*$.

We first describe two transformations.

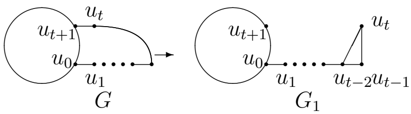

Figure 4.2. Graphs in Lemma 4.1

Lemma 4.1. (Transformation 4 [9]) Let G, G_1 be the graphs as shown in Figure 4.2, where $d_G(u_i) = 2$ for any $1 \leq i \leq t$ and $t \geq 2$. Then $\sigma(G) \geq \sigma(G_1)$ and the equality holds if and only if $t = 2$ and $u_3 = u_0$.

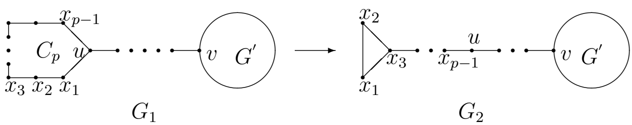

Figure 4.3. Graphs in Lemma 4.2

Lemma 4.2. (Transformation 5 [9]) Let G_1 and G_2 be the graphs as shown in Figure 4.3, where C_p and the path joining u and v are pending, $G_1 = G_2 - x_1u + x_3x_1$ and $p \geq 4$. Then $\sigma(G_1) > \sigma(G_2)$.

Lemma 4.3. For any tricyclic graph G in $\mathcal{A}(p, q, l, r)$, $\mathcal{B}(p, q, l, t, r)$ and $\mathcal{C}(p, q, l, s, t, r)$, there is a graph $H \in \mathcal{D}(p, q, l, r) \cup \mathcal{E}(p, q, l)$ such that $\sigma(G) > \sigma(H)$.

Proof. We distinguish the following three cases.

Case 1. $G \in \mathcal{A}(p, q, l, r)$, as shown in Figure 1.4 ($\mathcal{A}$).

Then there exist four pending paths P_1, P_2, P_3, P_4 of G joining two vertices of degree 3 (see u and v in Figure 4.4). Since $n \geq 11$, we can assume that P_4 has length at least 4 without loss of generality. Then by Transformation 4 and Lemma 4.1, there exists a graph H in $\mathcal{D}(p, q, l, r)$ such that $\sigma(G) > \sigma(H)$. (See Figure 4.4, which is the case that $n = 11$).

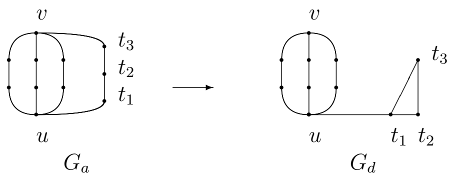

Figure 4.4.

Case 2. $G \in \mathcal{B}(p,q,l,t,r)$, as shown in Figure 1.4 ($\mathcal{B}$).

Then there exist six pending paths of G joining two vertices of degree 3 (see u_1, u_2, v_1, v_2 in Figure 4.5). Since $n \geq 11$, there exists one path among the six pending paths with length at least 3. If there exists one path with length at least 4, there exists a graph H in $\mathcal{D}(p,q,l,r)$ such that $\sigma(G) > \sigma(H)$. Suppose that all the pending paths have length at most 3. Then $11 \leq n \leq 16$. Then by Transformation 4 and Lemma 4.1, we can find a graph H in $\mathcal{D}(p,q,l,r)$ or $\mathcal{E}(p,q,l)$ such that $\sigma(G) > \sigma(H)$ for any $11 \leq n \leq 16$ as shown in Figure 4.5(where $\sigma(G_{b1}) > \sigma(G_{b2}) > \sigma(G_e)$).

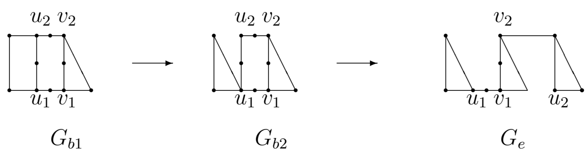

Figure 4.5.

Case 3. $G \in \mathcal{C}(p,q,l,s,t,r)$, as shown in Figure 1.4 ($\mathcal{C}$).

Then there exist six pending paths of G joining two vertices of degree 3 (see u_1, u_2, u_3, u_4 in Figure 4.6). Since $n \geq 11$, there exists one path among the six pending paths with length at least 3. If there exists one path with length at least 4, there exists a graph H in $\mathcal{D}(p,q,l,r)$ such that $\sigma(G) > \sigma(H)$. Suppose that all the pending paths have length at most 3. Then $11 \leq n \leq 16$. Then by Transformation 4 and Lemma 4.1, we can find a graph H in $\mathcal{D}(p,q,l,r)$ or $\mathcal{E}(p,q,l)$ such that $\sigma(G) > \sigma(H)$ for any $11 \leq n \leq 16$ as shown in Figure 4.6(where $\sigma(G_{c1}) > \sigma(G_{c2}) > \sigma(G_d)$).

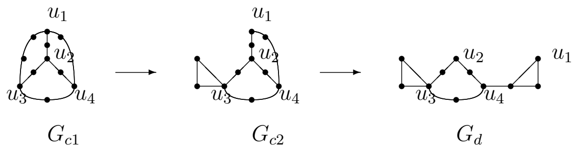

Figure 4.6.

Therefore, to determine the smallest Merrifield–Simmons index in tricyclic graphs and give the extremal graph, we only need to consider the graphs in $\mathcal{D}(p,q,l,r) \cup \mathcal{E}(p,q,l)$.

Now, we consider the graph in $\mathcal{D}(p,q,l,r)$ with $n \geq 11$ (see Figure 4.7.)

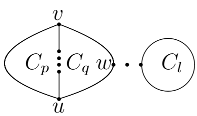

Figure 4.7.

By Lemma 4.1, it is easy to get the following lemma.

Lemma 4.4. Let G be in $\mathcal{D}(p,q,l,r)$ as shown in Figure 4.7 satisfying one of conditions: (1) $p \geq 5$; (2) the pending path joining w and v(or u) has length at least 3; (3) there exists one pending path joining u and v with length exactly 3 and the pending path joining w and v(or u) has length exactly 2. Then there exists a graph $H \in \mathcal{E}(p,q,l)$ such that $\sigma(G) > \sigma(H)$.

It is easy to check that all graphs in $\mathcal{D}(p,q,l,t)$ not satisfying any conditions in Lemma 4.4 are the 12 graphs depicted in Fig. 4.8.

Lemma 4.5. H_1 is the graph with the smallest Merrifield–Simmons index in $\{H_1, \cdots, H_9\}$, $\sigma(H_1) = 22f(n-6) + 14f(n-7)$ and there exists a graph H in $\mathcal{E}(p,q,l)$ such that $\sigma(H_i) > \sigma(H)$ for each $10 \leq i \leq 12$.

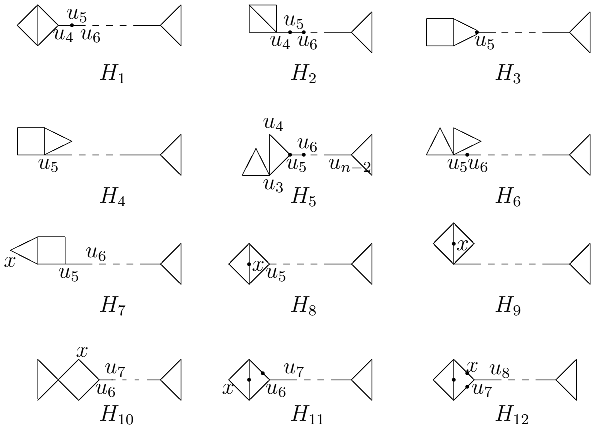

Figure 4.8.

Proof. By Lemma 4.1, $\sigma(H_5) < \sigma(H_3)$ and $\sigma(H_5) < \sigma(H_4)$. By Proposition 1.1(1)-(5),

$$\begin{aligned}
\sigma(H_1) &= \sigma(H_1 - u_5) + \sigma(H_1 - \{u_4, u_5, u_6\}) \\
&= 6(f(n-4) + f(n-6)) + 4(f(n-5) + f(n-7)) \\
&= 22f(n-6) + 14f(n-7)\ . \\
\sigma(H_5) &= \sigma(H_5 - u_5) + \sigma(H_5 - \{u_3, u_4, u_5, u_6\}) \\
&= 7(f(n-4) + f(n-6)) + 3(f(n-5) + f(n-7)) \\
&= 24f(n-6) + 13f(n-7) > \sigma(H_1)\ . \\
\sigma(H_1) - \sigma(H_2) &= \sigma(H_1 - u_5) + \sigma(H_1 - \{u_4, u_5, u_6\}) \\
&- \sigma(H_2 - u_5) - \sigma(H_2 - \{u_4, u_5, u_6\}) \\
&= \sigma(H_1 - \{u_4, u_5, u_6\}) - \sigma(H_2 - \{u_4, u_5, u_6\}) < 0
\end{aligned}$$

by Proposition 1.1 (3).

By the same method as above, we have $\sigma(H_7) < \sigma(H_8) < \sigma(H_9)$ (by Proposition 1.1(4) on x), $\sigma(H_5) = \sigma(H_7)$ (by Proposition 1.1(4) on u_5), and $\sigma(H_5) < \sigma(H_6)$ (by Proposition 1.1(4) on u_6). Let $H_1' = H_{10} - u_6u_7 + xu_7$, $H_2' = H_{11} - u_6u_7 + xu_7$ and $H_3' =$

$H_{12}-u_7u_8+xu_8$. By the above method and Lemma 1.1, $\sigma(H_{10}) > \sigma(H_1')$, $\sigma(H_{11}) > \sigma(H_2')$ and $\sigma(H_{12}) > \sigma(H_3')$. By Lemma 4.1, there exist G_1, G_2 and G_3 in $\mathcal{E}(p,q,l)$ such that $\sigma(H_i') > \sigma(G_i)$ for each $1 \le i \le 3$. The proof is completed.

Finally, we consider the tricyclic graph G in $\mathcal{E}(p,q,l)$.

By Lemma 4.1 and Lemma 4.2, we only need to consider the following three graphs H_{13}, H_{14} and H_{15} (as shown in Figure 4.9).

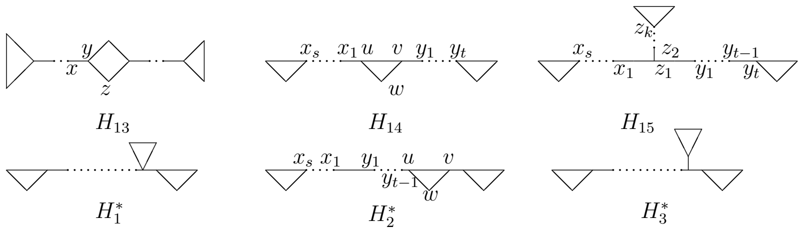

Figure 4.9.

Lemma 4.6. For any tricyclic graph G in $\mathcal{E}(p,q,l)$ with $n \ge 11$, we have $\sigma(G) \ge \sigma(H_3^*) = 57f(n-8) + 34f(n-9)$ and the equality holds if and only if $G \cong H_3^*$.

Proof. It suffices to prove that $\sigma(H_j) \ge \sigma(H_3^*)$ for any $13 \le j \le 15$ and the equality holds if and only if $H_j \cong H_3^*$.

Let $H = H_{13} - xy + xz$. By Proposition 1.1(4) on x and Lemma 1.1, $\sigma(H) < \sigma(H_{13})$. By Lemma 4.1, $\sigma(H_{15}) < \sigma(H)$, where $k = 1$. By Proposition 1.1(4)-(6) on w,

$$\begin{aligned}
& \sigma(H_2^*) - \sigma(H_{14}) \\
= \; & \sigma(H_2^* - \{w,u,v\}) - \sigma(H_{14} - \{w,u,v\}) \\
= \; & 4(f(s+t+2) + f(s+t)) - (f(s+3) + f(s+1))(f(t+3) + f(t+1)) \\
= \; & 4(f(s+3)f(t) + f(s+2)f(t-1) + f(s+t)) \\
- \; & (f(s+3) + f(s+1))(4f(t) + 3f(t-1)) \\
= \; & 4f(t-1)(f(s+2) + f(s)) - 3f(t-1)(f(s+3) + f(s+1)) \\
= \; & -5f(t-1)f(s-1) \le 0 \; .
\end{aligned}$$

Then $\sigma(H_2^*) \leq \sigma(H_{14})$ and the equality holds if and only if $H_2^* \cong H_{14}$.

Without loss of generality, suppose that $s \geq t \geq k$ in H_{15}. Let $H = H_{15} - \{x_1z_1, z_1y_1, y_{t-1}y_t\} + \{x_1y_1, y_{t-1}z_1, z_1y_t\}$ and H_0 the component of $H_{15} - z_1$ containing z_2. Then when $k = 1$, $H = H_1^*$. Let $m = 1$ if $k = 1$ and $m = \sigma(H_0 - z_2)$ if $k \geq 2$. Then $m < \sigma(H_0)$. By Proposition 1.1(4)-(6) on z_1 ,

$$\begin{aligned}
& \sigma(H) - \sigma(H_{15}) \\
= \ & \sigma(H - z_1) - \sigma(H_{15} - z_1) + \sigma(H - \{z_1, x_1, y_1\}) - \sigma(H_{15} - \{z_1, y_t, y_{t-1}\}) \\
= \ & \sigma(H_0)[4f(s+t+2) + 4f(s+t) - (f(s+3) + f(s+1))(f(t+3) + f(t+1))] \\
+ \ & m[3f(s+t+1) + 3f(s+t-1) - (f(s+2) + f(s))(f(t+2) + f(t))] \\
= \ & -5f(t-1)f(s-1)\sigma(H_0) + m[3f(s+2)f(t) + 3f(s+1)f(t-1) \\
+ \ & 3f(s)f(t) + 3f(s-1)f(t-1) - (f(s+2) + f(s))(3f(t) + f(t-1))] \\
= \ & -5f(t-1)f(s-1)\sigma(H_0) + 5mf(t-1)f(s-1) \leq 0 \ .
\end{aligned}$$

Then $\sigma(H) \leq \sigma(H_{15})$ and the equality holds if and only if $H \cong H_{15}$. When $k \geq 2$, by the above method, $\sigma(H_3^*) \leq \sigma(H)$ and the equality holds if and only if $H_3^* \cong H$.

By Proposition 1.1(1)–(6),

$$\begin{aligned}
\sigma(H_1^*) &= 57f(n-8) + 39f(n-9) \\
\sigma(H_2^*) &= 56f(n-8) + 37f(n-9) \\
\sigma(H_3^*) &= 57f(n-8) + 34f(n-9) \ .
\end{aligned}$$

Then $\sigma(H_3^*) < \sigma(H_2^*) < \sigma(H_1^*)$.

By Lemma 4.5, $\sigma(H_1) = 22f(n-6) + 14f(n-7) > \sigma(H_3^*)$.

Thus the proof of Theorem 4.1 is completed.

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