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The Merrifield–Simmons index in $(n, n+1)$-graphs

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A $(n, n+1)$-graph G is a connected simple graph with n vertices and $n+1$ edges. In this paper, we determine the upper bound for the Merrifield–Simmons index in $(n, n+1)-$graphs in terms of the order n, and characterize the $(n, n+1)-$graph with the largest Merrifield–Simmons index.

KEY WORDS: $(n, n+1)$-graph, Merrifield–Simmons index

1. Introduction

Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. For any $v \in V$, $N_G(v) = \{u|uv \in E(G)\}$ denotes the neighbors of v, and $d_G(v) = |N_G(v)|$ is the degree of v in G; $N_G[v] = \{v\} \cup N_G(v)$. A leaf is a vertex of degree one and a stem is a vertex adjacent to at least one leaf. Let $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. $W \subseteq V(G)$, $G - W$ denotes the subgraph of G obtained by deleting the vertices of W and the edges incident with them. If a graph G has components $G_1, G_2, \ldots, G_t$, then G is denoted by $\bigcup_{i=1}^{t} G_i$. P_n denotes the path on n vertices, C_n is the cycle on n vertices, and S_n is the star consisting of one center vertex adjacent to $n - 1$ leaves.

For a graph $G = (V, E)$, a subset $S \subseteq V$ is called independent if no two vertices of S are adjacent in G. The set of independent sets in G is denoted by $I(G)$. The empty set is an independent set. The number of independent sets in G, denoted by $i(G)$, is called the Merrifield–Simmons index or σ-index in theoretical chemistry.

The Merrifield–Simmons index [1–3] is one of the topological indices whose mathematical properties were studied in some detail [4–12] whereas its applicability for QSPR and QSAR was examined to a much lesser extent; in [2] it was shown that $i(G)$ is correlated with the boiling points.

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For the Merrifield–Simmons index, bounds for several classes of graphs were given. For instance, it was observed in [4] that the star S_n and the path P_n have the largest and the smallest Fibonacci number among all trees with n vertices, respectively; $i(S_n) = 2^{n-1} + 1$ and $i(P_n) = f(n+2)$, where $f(0) = 0, f(1) = 1$ and $f(n) = f(n-1) + f(n-2)$ for $n \geqslant 2$ denotes the sequence of Fibonacci numbers. This is perhaps why some authors [4] called $i(G)$ the Fibonacci number of the graph. Pedersen and Vestergaard [12] gave upper and lower bounds in unicyclic graphs in terms of order and characterized the extremal graphs, [11] determined the tree with the largest Merrifield–Simmons index among all trees with n vertices and with diameter k. For further details on the Merrifield–Simmons index (see the book [2], the papers [4–12] and the references cited therein).

Let x and y be two vertices in G. The set of independent sets in which contain the vertex x is denoted by $I_x(G)$, while $I_{-x}(G)$ denotes the set of independent sets which do not contain x. Then

(i) $i(G) = |I_{-x}(G)| + |I_x(G)| = i(G - \{x\}) + i(G - N_G[x])$.

(ii) If x and y are not adjacent in G, then
$i(G) = i(G - \{x, y\}) + i(G - \{x\} \cup N_G[y]) + i(G - \{y\} \cup N_G[x]) + i(G - N_G[x] \cup N_G[y])$.

(iii) If x and y are adjacent in G, then
$i(G) = i(G - \{x, y\}) + i(G - N_G[y]) + i(G - N_G[x])$.

(iv) If G is a graph with components $G_1, G_2, G_3, \ldots, G_k$, then $i(G) = \prod_{i=1}^{k} i(G_i)$.

(v) $i(P_n) = f(n+2)$ for any $n \in \mathbb{N}$;
$i(C_n) = f(n-1) + f(n+1)$ for any $n \geqslant 3$.

In this paper, we investigate the Merrifield–Simmons index of $(n, n+1)-$graphs, i.e., connected simple graphs with n vertices and $n+1$ edges. We characterize the $(n, n+1)-$graph among all $(n, n+1)-$graphs with the largest Merrifield–Simmons index.

Let $\mathcal{G}(n, n+1)$ be the set of simple connected graphs with n vertices and $n+1$ edges. For any graph $G \in \mathcal{G}(n, n+1)$, there are two cycles C_p and C_q in G. As in [13], we divide all the $(n, n+1)-$graphs with two cycles of lengths p and q into three classes.

(1) $\mathcal{A}(p, q)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have only one common vertex.

(2) $\mathcal{B}(p, q)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have no common vertex.

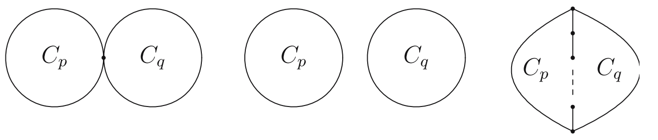

Figure 1. The induced subgraphs of vertices on the cycles of an (n,n+1)-graph

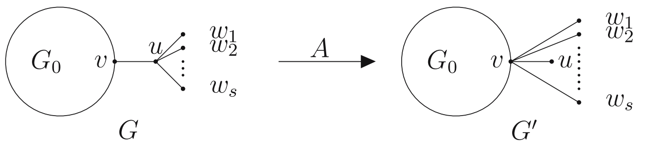

Figure 2. Transformation A.

(3) $\mathcal{C}(p, q, l)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have a common path of length l.

Note that the induced subgraph of vertices on the cycles of $G \in \mathcal{A}(p, q)$ (or $\mathcal{B}(p, q)$, $\mathcal{C}(p, q, l)$) is showed in figure 1(a) (or (b),(c)), and $\mathcal{C}(p, q, l) = \mathcal{C}(p, p+q-2l, p-l) = \mathcal{C}(p+q-2l, q, q-l)$.

2. Two transformations

Before our main results, we give two transformations which will increase the Merrifield–Simmons index as follows:

Transformation A. Let uv be an edge G, $N_G(u) = \{v, w_1, w_2, \ldots, w_s\}$, and $w_1, w_2, \ldots, w_s$ are leaves. $G' = G - \{vw_1, vw_2, \ldots, vw_s\} + \{uw_1, uw_2, \ldots, uw_s\}$, as shown in figure 2.

Lemma 2.1. Let G' be obtained from G by transformation A, then

$$i(G') > i(G).$$

Proof. Let $G_0 = G - \{u, w_1, w_2, \ldots, w_s\}$. By the definition of the number of independent sets, we have

$$\begin{aligned}
i(G) &= |I_{-v}(G)| + |I_v(G)| \\
&= i(G - \{v\}) + i(G - N_G[v]) \\
&= (1 + 2^s) \cdot i(G_0 - \{v\}) + 2^s \cdot i(G_0 - N_{G_0}[v]) \\
i(G') &= 2^{s+1} \cdot i(G_0 - \{v\}) + i(G_0 - N_{G_0}[v]).
\end{aligned}$$

Then

$$\Delta = i(G') - i(G)$$
$$= (2^s - 1) \cdot (i(G_0 - \{v\}) - i(G_0 - N_{G_0}[v])) > 0$$

since $\varphi(X) = X \cup \{v\}$ is an injection from $I(G_0 - N_{G_0}[v])$ to $I(G_0 - \{v\})$. Therefore, $i(G') > i(G)$.

Remark. Repeating transformation A, any $(n, n+1)-$graph can be changed into an $(n, n+1)-$graph such that all the edges not on the cycles are pendant edges.

Transformation B. Let u and v be two vertices in G. $u_1, u_2, \ldots, u_s$ are the leaves adjacent to $u, v_1, v_2, \ldots, v_t$ are the leaves adjacent to v. $G' = G - \{uu_1, uu_2, \ldots, uu_s\} + \{vu_1, vu_2, \ldots, vu_s\}$, $G''=G - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\}$ (figure 3).

Lemma 2.2. Let G' and G'' be obtained from G by transformation B, then either $i(G') > i(G)$ or $i(G'') > i(G)$.

Proof. Let $G_0 = G - \{u_1, u_2, \ldots, u_s, v_1, v_2, \ldots, v_t\}$.

(i) If u, v are not adjacent in G, then, by the definition of the number of independent sets, we have

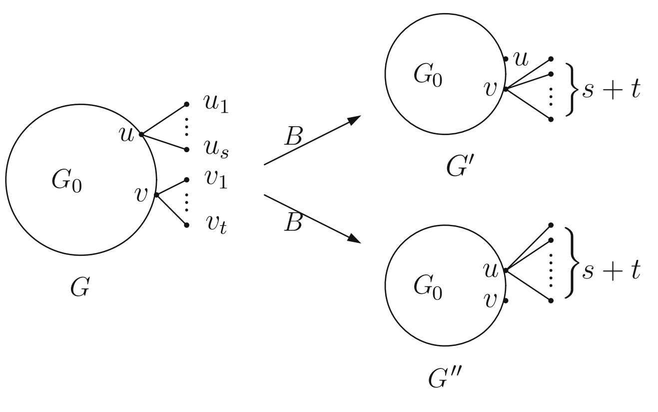

Figure 3. Transformation B.

$$\begin{aligned}
i(G) &= i(G - \{v\}) + i(G - N_G[v]) \\
&= 2^{s+t} i(G_0 - \{u, v\}) + 2^t i(G_0 - \{v\} \cup N_{G_0}[u]) \\
&\quad + 2^s i(G_0 - \{u\} \cup N_{G_0}[v]) + i(G_0 - N_{G_0}[v] \cup N_{G_0}[u]) \\
i(G') &= i(G - \{v\}) + i(G - N_G[v]) \\
&= 2^{s+t} (i(G_0 - \{u, v\}) + i(G_0 - \{v\} \cup N_{G_0}[u])) \\
&\quad + i(G_0 - \{u\} \cup N_{G_0}[v]) + i(G_0 - N_{G_0}[v] \cup N_{G_0}[u]) \\
i(G'') &= i(G - \{v\}) + i(G - N_G[v]) \\
&= 2^{s+t} (i(G_0 - \{u, v\}) + i(G_0 - \{u\} \cup N_{G_0}[v])) \\
&\quad + i(G_0 - \{v\} \cup N_{G_0}[u]) + i(G_0 - N_{G_0}[v] \cup N_{G_0}[u]) \\
\Delta_1 &= i(G') - i(G) \\
&= (2^s - 1)(2^t i(G_0 - \{v\} \cup N_{G_0}[u]) - i(G_0 - \{u\} \cup N_{G_0}[v])) \\
\Delta_2 &= i(G'') - i(G) \\
&= (2^t - 1)(2^s i(G_0 - \{u\} \cup N_{G_0}[v]) - i(G_0 - \{v\} \cup N_{G_0}[u])).
\end{aligned}$$

If $\Delta_1 = i(G') - i(G) \leqslant 0$, then $i(G_0 - \{u\} \cup N_{G_0}[v]) \geqslant 2^t i(G_0 - \{v\} \cup N_{G_0}[u])$.
So, $\Delta_2 = i(G'') - i(G) \geqslant (2^t - 1)(2^{s+t} - 1) i(G_0 - \{v\} \cup N_{G_0}[u]) > 0$.

(ii) If u, v are adjacent in G, then

$$\begin{aligned}
i(G) &= 2^{s+t} i(G_0 - \{u, v\}) + 2^t i(G_0 - N_{G_0}[u]) + 2^s i(G_0 - N_{G_0}[v]) \\
i(G') &= i(G - \{v\}) + i(G - N_G[v]) \\
&= 2^{s+t} (i(G_0 - \{u, v\}) + i(G_0 - N_{G_0}[u])) + i(G_0 - N_{G_0}[v]) \\
i(G'') &= i(G - \{u\}) + i(G - N_G[u]) \\
&= 2^{s+t} (i(G_0 - \{u, v\}) + i(G_0 - N_{G_0}[v])) + i(G_0 - N_{G_0}[u]) \\
\Delta_1 &= i(G') - i(G) \\
&= (2^s - 1)(2^t i(G_0 - N_{G_0}[u]) - i(G_0 - N_{G_0}[v])) \\
\Delta_2 &= i(G'') - i(G) \\
&= (2^t - 1)(2^s i(G_0 - N_{G_0}[v]) - i(G_0 - N_{G_0}[u])).
\end{aligned}$$

If $\Delta_1 = i(G') - i(G) \leqslant 0$, then $i(G_0 - N_{G_0}[v]) \geqslant 2^t i(G_0 - N_{G_0}[u])$.
So, $\Delta_2 = i(G'') - i(G) \geqslant (2^t - 1)(2^{s+t} - 1) i(G_0 - N_{G_0}[u]) > 0$.
The proof is completed.

Remark. Repeating transformation B, any $(n, n+1)-$graph can be changed into an $(n, n+1)-$graph such that all the pendant edges are attached to the same vertex.

3. The graph with the largest Merrifield–Simmons index in $\mathcal{A}(p, q)$

In this section, we will find the $(n, n+1)-$graph with the largest Merrifield–Simmons index in $\mathcal{A}(p, q)$.

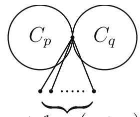

Figure 4. The graph $S_n(p,q)$.

Let $S_n(p,q)$ be a graph in $\mathcal{A}(p,q)$ such that $n+1-(p+q)$ pendent edges are attached to the common vertex of C_p and C_q (see figure 4).

Theorem 3.1. If $G \in \mathcal{A}(p,q)$, then $i(G) \leqslant i(S_n(p,q)$ with the equality if and only if $G \cong S_n(p,q)$.

Proof. First, repeating the transformations A and B on graph G, we can get a graph G' such that all the edges not on the cycles are the pendant edges attached to the same vertex v. By lemmas 2.1 and 2.2, we have $i(G) \leqslant i(G')$ with the equality if and only if all the edges not on the cycles are also the pendant edges attached to the same vertex in G. If $G' \ncong S_n(p,q)$, then $v \neq u$, where u is the common vertex of C_p and C_q.

Without loss of the generality, we assume that v is on the cycle C_p and the distance $d(u,v) = k-1$.

(i) If u and v are not adjacent (i.e., $k > 1$), then

$$\begin{aligned}
&i(S_n(p,q)) - i(G') \\
&= i(S_n(p,q) - \{v,u\}) + i(S_n(p,q) - \{v\} \cup N_{S_n(p,q)}[u]) + i(S_n(p,q) \\
&\quad -\{u\} \cup N_{S_n(p,q)}[v]) + i(S_n(p,q) - N_{S_n(p,q)}[v] \cup N_{S_n(p,q)}[u]) \\
&\quad -i(G' - \{v,u\}) - i(G' - \{v\} \cup N_{G'}[u]) - i(G' - \{u\} \cup N_{G'}[v]) \\
&\quad -i(G' - N_{G'}[v] \cup N_{G'}[u])) \\
&= i(S_n(p,q) - \{v\} \cup N_{S_n(p,q)}[u]) + i(S_n(p,q) - \{u\} \cup N_{S_n(p,q)}[v]) \\
&\quad -i(G' - \{v\} \cup N_{G'}[u]) - i(G' - \{u\} \cup N_{G'}[v]) \\
&= i(P_{k-3} \cup P_{p-k-1} \cup P_{q-3}) + 2^{n+1-p-q} i(P_{k-3} \cup P_{p-k-1} \cup P_{q-1}) \\
&\quad -2^{n+1-p-q} i(P_{k-3} \cup P_{p-k-1} \cup P_{q-3}) - i(P_{k-3} \cup P_{p-k-1} \cup P_{q-1}) \\
&= (2^{n+1-p-q} - 1)(i(P_{k-3} \cup P_{p-k-1} \cup P_{q-1}) \\
&\quad -i(P_{k-3} \cup P_{p-k-1} \cup P_{q-3})) \geqslant 0
\end{aligned}$$

with the equality if and only if $n = p+q-1$, and $G' \cong S_n(p,q)$.

(ii) If u and v are adjacent (i.e., $k = 1$), then

$$\begin{aligned}
&i(S_n(p,q)) - i(G') \\
&\quad = i(S_n(p,q) - \{v,u\}) + i(S_n(p,q) - N_{S_n(p,q)}[u]) + i(S_n(p,q) \\
&\qquad - N_{S_n(p,q)}[v]) - i(G' - \{v,u\}) - i(G' - N_{G'}[u]) - i(G' - N_{G'}[v]) \\
&\quad = i(S_n(p,q) - N_{S_n(p,q)}[u]) + i(S_n(p,q) - N_{S_n(p,q)}[v]) \\
&\qquad - i(G' - N_{G'}[u]) - i(G' - N_{G'}[v]) \\
&\quad = i(P_{p-3} \cup P_{q-3}) + 2^{n+1-p-q} i(P_{p-3} \cup P_{q-1}) \\
&\qquad - 2^{n+1-p-q} i(P_{p-3} \cup P_{q-3}) - i(P_{p-3} \cup P_{q-1}) \\
&\quad = (2^{n+1-p-q} - 1)(i(P_{p-3} \cup P_{q-1}) - i(P_{p-3} \cup P_{q-3})) \\
&\quad \geqslant 0
\end{aligned}$$

with the equality if and only if $n = p + q - 1$, and $G' \cong S_n(p,q)$.

Given $p \geqslant 3$ and $q \geqslant 3$, from the theorem above, we know $S_n(p,q)$ is the unique graph with the largest Merrifield–Simmons index in $\mathcal{A}(p,q)$.

Lemma 3.2. $i(S_n(p,q)) = 2^{n+1-(p+q)} f(p+1) f(q+1) + f(p-1) f(q-1)$.

Proof. Let u be the common vertex of C_p and C_q in $S_n(p,q)$. Then we have

$$\begin{aligned}
i(S_n(p,q)) &= i(S_n(p,q) - \{u\}) + i(S_n(p,q) - N_{S_n(p,q)}[u]) \\
&= 2^{n+1-(p+q)} i(P_{p-1} \cup P_{q-1}) + i(P_{p-3} \cup P_{q-3}) \\
&= 2^{n+1-(p+q)} f(p+1) f(q+1) + f(p-1) f(q-1).
\end{aligned}$$

Lemma 3.3.

(i) If $p > 3$, then $i(S_n(p,q)) < i(S_n(p-1,q))$;

(ii) If $q > 3$, then $i(S_n(p,q)) < i(S_n(p,q-1))$.

Proof. From the symmetry of p and q, we only need to prove (i).

If $p > 3$, then by lemma 3.2 we have

$$\begin{aligned}
\Delta &= i(S_n(p-1,q)) - i(S_n(p,q)) \\
&= 2^{n+2-(p+q)} f(p) f(q+1) + f(p-2) f(q-1) \\
&\quad - 2^{n+1-(p+q)} f(p+1) f(q+1) - f(p-1) f(q-1) \\
&= 2 \times 2^{n+1-(p+q)} f(p) f(q+1) + f(p-2) f(q-1) \\
&\quad - 2^{n+1-(p+q)} (f(p) + f(p-1)) f(q+1) - (f(p-2) + f(p-3)) f(q-1) \\
&= 2^{n+1-(p+q)} (f(p) - f(p-1)) f(q+1) - f(p-3) f(q-1) \\
&= 2^{n+1-(p+q)} f(p-2) f(q+1) - f(p-3) f(q-1) \\
&= 2^{n+1-(p+q)} (f(p-3) + f(p-4)) f(q+1) - f(p-3) f(q-1) \\
&= 2^{n+1-(p+q)} f(p-4) f(q+1) + f(p-3)(2^{n+1-(p+q)} f(q+1) - f(q-1)) \\
&> 0
\end{aligned}$$

From theorem 3.1 and lemma 3.3, we know

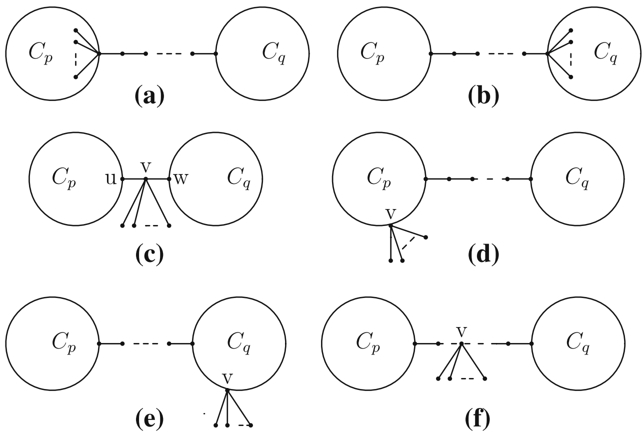

Figure 5. (a) $T_n^r(p, q)$, (b) $T_n^r(q, p)$, and (c) $T_n(p, q)$.

Theorem 3.4. For all $p \geqslant 3$ and $q \geqslant 3$, $S_n(3,3)$ is the unique graph with the largest Merrifield–Simmons index among $\mathcal{A}(p, q)$.

4. The graph with the largest Merrifield–Simmons index in $\mathcal{B}(p, q)$

In this section, we will find the $(n, n+1)-$graph with the largest Merrifield–Simmons index in $\mathcal{B}(p, q)$.

Let $T_n^r(p, q)$ be the $(n, n+1)-$graph obtaining from connecting C_p and C_q by a path of length r and the other $n+1-p-q-r$ edges are all attached to the common vertex of the path and C_p (see figure 5(a)). And $T_n^r(q, p)$ is showed in figure 5(b).

Theorem 4.1. If $G \in \mathcal{B}(p, q)$, the length of the shortest path connecting C_p and C_q is r, then either as follows:

(i) $i(G) \leqslant i(T_n^r(p, q))$ with the equality if and only if $G \cong T_n^r(p, q)$; or

(ii) $i(G) \leqslant i(T_n^r(q, p))$ with the equality if and only if $G \cong T_n^r(q, p)$; or

(iii) $i(G) \leqslant i(T_n(p, q))$ with the equality if and only if $G \cong T_n(p, q)$, where $T_n(p, q)$ is the $(n, n+1)-$graph obtaining from connecting C_p and C_q by a path uvw of length 3 and the other $n-p-q-1$ edges are all attached to the vertex w of the path, as showed in figure 5(c).

Proof. Let $W = v_1v_2, \ldots, v_rv_{r+1}$ be the shortest path connecting C_p and C_q, and v_1 the common vertex W and C_p, v_{r+1} the common vertex W and C_q.

Repeating the transformations A and B on graph G, we can get a graph G' in figure 5 such that all the edges not on the cycles are the pendant edges attached to the same vertex v. By lemmas 2.1 and 2.2, we have $i(G) \leqslant i(G')$ with the equality if and only if all the edges not on the cycles are also the pendant edges attached to the same vertex in G.

Case I. v is on the cycle C_p (as showed in figure 5(d)) and the distance $d(v_1, v) = k - 1$.

(i) If v_1 and v are not adjacent (i.e., $k > 1$), then

$$\begin{aligned}
&i(T_n^r(p,q)) - i(G') \\
&\quad = i(T_n^r(p,q) - \{v, v_1\}) + i(T_n^r(p,q) - \{v\} \cup N_{T_n^r(p,q)}[v_1]) + i(T_n^r(p,q) \\
&\qquad - \{v_1\} \cup N_{T_n^r(p,q)}[v]) + i(T_n^r(p,q) - N_{T_n^r(p,q)}[v] \cup N_{T_n^r(p,q)}[v_1]) \\
&\qquad - i(G' - \{v, v_1\}) - i(G' - \{v\} \cup N_{G'}[v_1]) - i(G' - \{v_1\} \cup N_{G'}[v]) \\
&\qquad - i(G' - N_{G'}[v] \cup N_{G'}[v_1]) \\
&\quad = i(T_n^r(p,q) - \{v\} \cup N_{T_n^r(p,q)}[v_1]) + i(T_n^r(p,q) - \{v_1\} \cup N_{T_n^r(p,q)}[v]) \\
&\qquad - i(G' - \{v\} \cup N_{G'}[v_1]) - i(G' - \{v_1\} \cup N_{G'}[v]) \\
&\quad = i(P_{k-3} \cup P_{p-k-1} \cup H_1) + 2^{n+1-(p+q+r)} i(P_{k-3} \cup P_{p-k-1} \cup H_2) \\
&\qquad - 2^{n+1-(p+q+r)} i(P_{k-3} \cup P_{p-k-1} \cup H_1) - i(P_{k-3} \cup P_{p-k-1} \cup H_2) \\
&\quad = (2^{n+1-(p+q+r)} - 1) \cdot (i(H_2) - i(H_1)) \cdot i(P_{k-3} \cup P_{p-k-1}) \\
&\quad \geqslant 0
\end{aligned}$$

with the equality if and only if $n = p + q + r - 1$, and then also $G' \cong T_n^r(p,q)$; where H_2 is the graph deleting v_1 from the subgraph of $T_n^r(p,q)$ consisting of C_q and W and $H_1 = H_2 - \{v_2\}$, and $i(H_2) < i(H_1)$ since any independent set in H_1 is also an independent set in H_2.

(ii) If v_1 and v are adjacent (i.e., $k = 1$), then

$$\begin{aligned}
&i(T_n^r(p,q)) - i(G') \\
&\quad = i(T_n^r(p,q) - \{v, v_1\}) + i(T_n^r(p,q) - N_{T_n^r(p,q)}[v_1]) + i(T_n^r(p,q) \\
&\qquad - N_{T_n^r(p,q)}[v]) - i(G' - \{v, v_1\}) - i(G' - N_{G'}[v_1]) - i(G' - N_{G'}[v]) \\
&\quad = i(T_n^r(p,q) - N_{T_n^r(p,q)}[v_1]) + i(T_n^r(p,q) - N_{T_n^r(p,q)}[v]) \\
&\qquad - i(G' - N_{G'}[v_1]) - i(G' - N_{G'}[v]) \\
&\quad = i(P_{p-3} \cup H_1) + 2^{n+1-(p+q+r)} i(P_{p-3} \cup H_2) \\
&\qquad - 2^{n+1-(p+q+r)} i(P_{p-3} \cup H_1) - i(P_{p-3} \cup H_2) \\
&\quad = (2^{n+1-(p+q+r)} - 1) \cdot (i(H_2) - i(H_1)) \cdot i(P_{p-3}) \\
&\quad \geqslant 0
\end{aligned}$$

with the equality if and only if $n = p + q + r - 1$, and then also $G' \cong T_n^r(p,q)$.

Case II. v is on the cycle C_q (as showed in figure 5(e)).

We can prove that $i(T_n^r(q,p)) \geqslant i(G)$ with the equality if and only if $G \cong T_n^r(q,p)$ as in the case I.

Case III. v is on the path W (as showed in figure 5(f)). Let $v = v_t$, $1 < t \leqslant r$.

$$
\begin{aligned}
& i(T_n(p,q)) - i(G') \\
&\quad = i(T_n(p,q) - \{u,w\}) + i(T_n(p,q) - \{w\} \cup N_{T_n(p,q)}[u]) \\
&\qquad + i(T_n(p,q) - \{u\} \cup N_{T_n(p,q)}[w]) + i(T_n(p,q) - N_{T_n(p,q)}[w] \cup N_{T_n(p,q)}[u]) \\
&\qquad - i(G' - \{v_1, v_{r+1}\}) - i(G' - \{v_{r+1}\} \cup N_{G'}[v_1]) \\
&\qquad - i(G' - \{v_1\} \cup N_{G'}[v_{r+1}]) - i(G' - N_{G'}[v_{r+1}] \cup N_{G'}[v_1]) \\
&\quad = i(P_{p-1} \cup P_{q-1} \cup S_{n-p-q}) + i(P_{p-3} \cup P_{q-1} \cup \overline{K_{n-1-p-q}}) \\
&\qquad + i(P_{p-1} \cup P_{q-3} \cup \overline{K_{n-1-p-q}}) + i(P_{p-3} \cup P_{q-3} \cup \overline{K_{n-1-p-q}}) \\
&\qquad - i(P_{p-1} \cup P_{q-1} \cup R_1) - i(P_{p-3} \cup P_{q-1} \cup R_2) \\
&\qquad - i(P_{p-1} \cup P_{q-3} \cup R_3) - i(P_{p-3} \cup P_{q-3} \cup R_4),
\end{aligned}
$$

where $R_1 = G' - C_p \cup C_q$, $R_2 = R_1 - \{v_2\}$, $R_3 = R_1 - \{v_r\}$ and $R_4 = R_1 - \{v_2, v_r\}$.

Since $i(R_1) \leqslant i(S_{n-p-q})$, $i(R_2) \leqslant i(\overline{K_{n-1-p-q}})$, $i(R_3) \leqslant i(\overline{K_{n-1-p-q}})$ and $i(R_4) \leqslant i(\overline{K_{n-1-p-q}})$, with the equality if and only if $v_2 = v_t = v_r$, i.e., $G' \cong T_n(p,q)$, $i(T_n(p,q)) \geqslant i(G')$.

Lemma 4.2.

(i) If $p \geqslant 5$, then $i(T_n(p,q)) < i(T_n(p-2,q))$;

(ii) If $q \geqslant 5$, then $i(T_n(p,q)) < i(T_n(p,q-2))$.

Proof. From the symmetry of p and q, we only need to prove (i). Let u, v be the vertices of degree 3 on the cycles. (u and v are not adjacent.)

$$
\begin{aligned}
& i(T_n(p-2,q)) - i(T_n(p,q)) \\
&\quad = i(T_n(p-2,q) - \{u,v\}) + i(T_n(p-2,q) - \{v\} \cup N_{T_n(p-2,q)}[u]) \\
&\qquad + i(T_n(p-2,q) - \{u\} \cup N_{T_n(p-2,q)}[v]) + i(T_n(p-2,q) \\
&\qquad - N_{T_n(p-2,q)}[v] \cup N_{T_n(p-2,q)}[u]) - i(T_n(p,q) - \{u,v\}) - i(T_n(p,q) \\
&\qquad - \{v\} \cup N_{T_n(p,q)}[u]) - i(T_n(p,q) - \{u\} \cup N_{T_n(p,q)}[v]) - i(T_n(p,q) \\
&\qquad - N_{T_n(p,q)}[v] \cup N_{T_n(p,q)}[u]) \\
&\quad = i(P_{p-3} \cup P_{q-1} \cup S_{n+2-p-q}) + i(P_{p-5} \cup P_{q-1} \cup \overline{K_{n+1-p-q}}) \\
&\qquad + i(P_{p-3} \cup P_{q-3} \cup \overline{K_{n+1-p-q}}) + i(P_{p-5} \cup P_{q-3} \cup \overline{K_{n+1-p-q}}) \\
&\qquad - i(P_{p-1} \cup P_{q-1} \cup S_{n-p-q}) - i(P_{p-3} \cup P_{q-1} \cup \overline{K_{n-1-p-q}}) \\
&\qquad - i(P_{p-1} \cup P_{q-3} \cup \overline{K_{n-1-p-q}}) - i(P_{p-3} \cup P_{q-3} \cup \overline{K_{n-1-p-q}})
\end{aligned}
$$

Since

$$
\begin{aligned}
& i(P_{p-3} \cup S_{n+2-p-q}) + i(P_{p-5} \cup \overline{K_{n+1-p-q}}) - i(P_{p-1} \cup S_{n-p-q}) \\
& \quad -i(P_{p-3} \cup \overline{K_{n-1-p-q}}) \\
& \quad = (1 + 2^{n+1-p-q}) f(p-1) + 2^{n+1-p-q} f(p-3) - (1 + 2^{n-1-p-q}) f(p+1) \\
& \quad\quad -2^{n-1-p-q} f(p-1) \\
& \quad = (1 + 4 \times 2^{n-1-p-q}) f(p-1) + 4 \times 2^{n-1-p-q}(f(p-1) - f(p-2)) \\
& \quad\quad -(1 + 2^{n-1-p-q})(2f(p-1) + f(p-2)) - 2^{n-1-p-q} f(p-1) \\
& \quad = 5 \times 2^{n-1-p-q}(f(p-1) - f(p-2)) - (f(p-1) + f(p-2)) \\
& \quad = 5 \times 2^{n-1-p-q} f(p-3) - 3f(p-3) - 2f(p-4) \\
& \quad > 0
\end{aligned}
$$

and

$$
\begin{aligned}
& i(P_{p-3} \cup \overline{K_{n+1-p-q}}) + i(P_{p-5} \cup \overline{K_{n+1-p-q}}) - i(P_{p-1} \cup \overline{K_{n-1-p-q}}) \\
& \quad -i(P_{p-3} \cup \overline{K_{n-1-p-q}}) \\
& \quad = 2^{n+1-p-q} f(p-1) + 2^{n+1-p-q} f(p-3) - 2^{n-1-p-q} f(p+1) \\
& \quad\quad -2^{n-1-p-q} f(p-1) \\
& \quad = 2^{n-1-p-q}(4 \times f(p-1) + 4 \times (f(p-1) - f(p-2)) - (2f(p-1) \\
& \quad\quad +f(p-2)) - f(p-1)) \\
& \quad = 5 \times 2^{n-1-p-q}(f(p-1) - f(p-2)) \\
& \quad > 0,
\end{aligned}
$$

we have $i(T_n(p-2, q)) > i(T_n(p, q))$.

From lemma 4.2, it is immediately that

Corollary 4.3.

(i) If p and q are odd, then $i(T_n(p, q)) \leqslant i(T_n(3, 3))$.

(ii) If p and q are even, then $i(T_n(p, q)) \leqslant i(T_n(4, 4))$.

(iii) If the parity of p and q is different, then $i(T_n(p, q)) \leqslant i(T_n(3, 4))$ with the equality if and only if $T_n(p, q)$ is one of $T_n(3, 3)$, $T_n(3, 4)$ and $T_n(4, 4)$.

Lemma 4.4. If $r > 1$, then

$$
\begin{aligned}
i(T_n^r(p, q) = {} & 2^{n+1-(p+q+r)} f(p+1) f(q+1) f(r+1) + f(p-1) f(q+1) f(r) \\
& +2^{n+1-(p+q+r)} f(p+1) f(q-1) f(r) + f(p-1) f(q-1) f(r-1);
\end{aligned}
$$

If $r = 1$, then $i(T_n^1(p, q)) = 2^{n-(p+q)} f(p+1)(f(q+1) + f(q-1)) + f(p-1) f(q+1)$.

Proof. Let u and v be the vertices with degree more than two on the cycles C_p and C_q, respectively; and $G = T_n^r(p, q)$.

If $r \geqslant 2$, u and v are not adjacent. Then

$$\begin{aligned} i(T_n^r(p,q)) &= i(G-\{u,v\})) + i(G-\{v\}\cup N_G[u]) \\ &\quad + i(G-\{u\}\cup N_G[v]) + i(G-N_G[u]\cup N_G[v]) \\ &= 2^{n+1-(p+q+r)} i(P_{p-1}\cup P_{q-1}\cup P_{r-1}) + i(P_{p-3}\cup P_{q-1}\cup P_{r-2}) \\ &\quad + 2^{n+1-(p+q+r)} i(P_{p-1}\cup P_{q-3}\cup P_{r-2}) + i(P_{p-3}\cup P_{q-3}\cup P_{r-3}) \\ &= 2^{n+1-(p+q+r)} f(p+1)f(q+1)f(r+1) + f(p-1)f(q+1)f(r) \\ &\quad + 2^{n+1-(p+q+r)} f(p+1)f(q-1)f(r) + f(p-1)f(q-1)f(r-1) \end{aligned}$$

If $r = 1$, then

$$\begin{aligned} i(T_n^1(p,q)) &= i(G-\{u\}) + i(G-N_G[u]) \\ &= 2^{n-(p+q)} i(P_{p-1}\cup C_q) + i(P_{p-3}\cup P_{q-1}) \\ &= 2^{n-(p+q)} f(p+1)(f(q+1)+f(q-1)) + f(p-1)f(q+1) \end{aligned}$$

Lemma 4.5. If $r > 1$, then
$i(T_n^r(p,q)) < i(T_n^{r-1}(p,q))$.

Proof. If $r > 2$, then

$$\begin{aligned} & i(T_n^{r-1}(p,q)) - i(T_n^r(p,q)) \\ &= 2\times 2^{n+1-(p+q+r)} f(p+1)f(q+1)f(r) + f(p-1)f(q+1)f(r-1) \\ &\quad + 2\times 2^{n+1-(p+q+r)} f(p+1)f(q-1)f(r-1) + f(p-1)f(q-1)f(r-2) \\ &\quad - 2^{n+1-(p+q+r)} f(p+1)f(q+1)f(r+1) - f(p-1)f(q+1)f(r) \\ &\quad - 2^{n+1-(p+q+r)} f(p+1)f(q-1)f(r) - f(p-1)f(q-1)f(r-1) \\ &= 2^{n+1-(p+q+r)} f(p+1)f(q+1)(f(r)-f(r-1)) \\ &\quad + f(p-1)f(q+1)(f(r-1)-f(r)) \\ &\quad + 2^{n+1-(p+q+r)} f(p+1)f(q-1)(f(r-1)-f(r-2)) \\ &\quad + f(p-1)f(q-1)(f(r-2)-f(r-1)) \\ &> 0. \end{aligned}$$

If $r = 2$, then

$$\begin{aligned} & i(T_n^1(p,q)) - i(T_n^2(p,q)) \\ &= 2^{n-(p+q)} f(p+1)(f(q+1)+f(q-1)) + f(p-1)f(q+1) \\ &\quad - 2^{n+1-(p+q+2)} f(p+1)f(q+1)f(3) - f(p-1)f(q+1)f(2) \\ &\quad - 2^{n+1-(p+q+2)} f(p+1)f(q-1)f(2) - f(p-1)f(q-1)f(1) \\ &= 2^{n+1-(p+q+2)} f(p+1)f(q-1) - f(p-1)f(q-1) \\ &> 0. \end{aligned}$$

For the graph $T_n^r(q,p)$, the similar results hold. From lemma 4.5, it is immediately that

Corollary 4.6. If $r > 1$, then $i(T_n^r(p,q)) < i(T_n^1(p,q))$ and $i(T_n^r(q,p)) < i(T_n^1(q,p))$.

Lemma 4.7.

(i) If $p > 3$, then $i(T_n^1(p,q)) < i(T_n^1(p-1,q))$;

(ii) If $q > 3$, then $i(T_n^1(p,q)) < i(T_n^1(p,q-1))$;

(iii) If $p > 3$, then $i(T_n^1(q,p)) < i(T_n^1(q,p-1))$;

(iv) If $q > 3$, then $i(T_n^1(q,p)) < i(T_n^1(q-1,p))$;

(v) If $r > 1$ or $p > 3$ or $q > 3$, then $i(T_n^r(p,q)) < i(T_n^1(3,3))$.

Proof.

(i)

$$\begin{aligned}
&i(T_n^1(p-1,q)) - i(T_n^1(p,q))\\
&\quad = 2^{n+1-(p+q)} f(p)(f(q+1)+f(q-1)) + f(p-2)f(q+1)\\
&\qquad -2^{n-(p+q)} f(p+1)(f(q+1)+f(q-1)) - f(p-1)f(q+1)\\
&\quad = 2^{n-(p+q)}(f(q+1)+f(q-1))(f(p)-f(p-1))\\
&\qquad -f(q+1)(f(p-1)-f(p-2))\\
&\quad = 2^{n-(p+q)}(f(q+1)+f(q-1))f(p-2) - f(q+1)f(p-3)\\
&\quad > 0,
\end{aligned}$$

(ii)

$$\begin{aligned}
&i(T_n^1(p,q-1)) - i(T_n^1(p,q))\\
&\quad = 2^{n+1-(p+q)} f(p+1)(f(q)+f(q-2)) + f(p-1)f(q)\\
&\qquad -2^{n-(p+q)} f(p+1)(f(q+1)+f(q-1)) - f(p-1)f(q+1)\\
&\quad = 2^{n+1-(p+q)} f(p+1)(f(q)+f(q-2)) + f(p-1)f(q)\\
&\qquad -2^{n-(p+q)} f(p+1)(f(q)+f(q-1)+f(q-2)\\
&\qquad +f(q-3)) - f(p-1)f(q+1)\\
&\quad = 2^{n-(p+q)} f(p+1)(f(q)+f(q-2)-f(q-1)-f(q-3))\\
&\qquad -f(p-1)(f(q+1)-f(q))\\
&\quad = 2^{n-(p+q)} f(p+1)(f(q-2)+f(q-4)) - f(p-1)(f(q-2)\\
&\qquad +f(q-4)+f(q-5))\\
&\quad > 2^{n-(p+q)} f(p+1)f(q-4) - 2f(p-1)f(q-4)\\
&\quad > 0
\end{aligned}$$

(iii) and (iv) can be proved similarly. (v) is immediate from (i)–(iv).

Now, we compare the Merrifield–Simmons indices of $T_n^1(3,3)$, $T_n(3,3)$, $T_n(3,4)$, and $T_n(4,4)$. It can be computed out easily that

$$i(T_n^1(3,3)) = 3 \times 2^{n-4} + 3 = 96 \times 2^{n-9} + 3.$$

$$i(T_n(3,3)) = 2^{n-3} + 9 = 64 \times 2^{n-9} + 9.$$

$$i(T_n(3,4)) = 7 \times 2^{n-6} + 15 = 56 \times 2^{n-9} + 15.$$

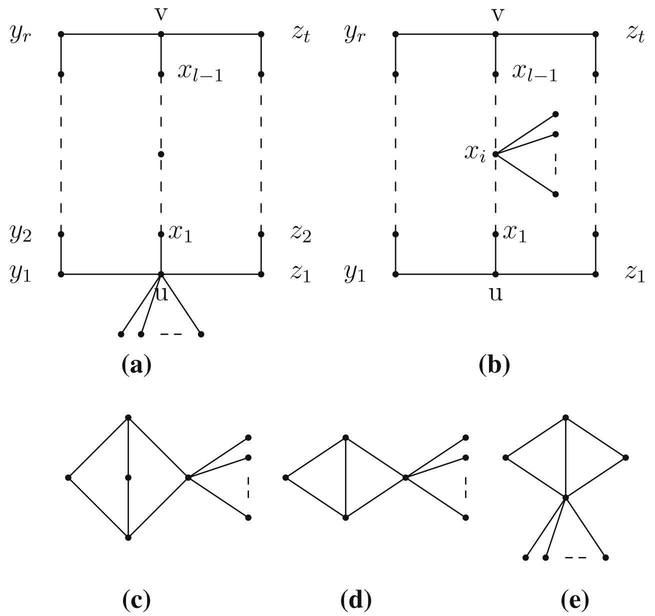

Figure 6.

$i(T_n(4,4)) = 49 \times 2^{n-9} + 25.$

Then $i(T_7^1(3,3)) > i(T_7(3,3))$, $i(T_8^1(3,3)) > i(T_8(3,4)) > i(T_8(3,3))$, and $i(T_n^1(3,3)) > i(T_n(3,3)) > i(T_n(3,4)) > i(T_n(4,4))$ for $n > 8$. So, we have

Theorem 4.8. The $T_n^1(3,3)$ is the unique graph with the largest Merrifield–Simmons index among all graphs in $\mathcal{B}(p,q)$ for all $p \geqslant 3$ and $q \geqslant 3$.

5. The graph with the largest Merrifield–Simmons index in $\mathcal{C}(p,q,l)$

In this section, we will find the $(n, n+1)-$graph with the largest Merrifield–Simmons index in $\mathcal{C}(p,q,l)$.

Let $\theta_n^l(p,q)$ be the graph obtaining from the graph in figure 1(c) by attaching $n+1+l-(p+q)$ to one of its vertices with degree 3 (see figure 6(a)).

Theorem 5.1. Let $G \in \mathcal{C}(p,q,l)$. Then $i(G) \leqslant i(G_0)$ with the equality if and only if $G \cong G_0$, where G_0 is one of graphs in figure 6(c), (d), and (e).

Proof. Let $W_1 = ux_1x_2\ldots x_{l-1}v$ be the common path of C_p and C_q of the graph G in Figure 6(a), $W_2 = uy_1y_2\ldots y_rv$ and $W_3 = uz_1z_2\ldots z_tv$ the other paths from u to v on C_p and C_q, respectively; $r = p-l-1$, $t = q-l-1$.

Table 1
The mapping $\rho\colon I(G') \to I(G'')$.

x_i	x_{i-1}	x_{i-2}	$\rho(B)$
0	0	0	B
0	0	1	B
0	1	0	B
1	0	0	B
1	0	1	$(B - \{x_i\}) \cup \{x_{i-1}\}$

Repeating the transformations A and B on graph G, we can get a graph $G' \in \mathcal{C}(p, q, l)$ such that all the edges not on the cycles are the pendant edges attached to the same vertex v_0. By lemmas 2.1 and 2.2, we have $i(G) \leqslant i(G')$ with the equality if and only if all the edges not on the cycles are also the pendant edges attached to the same vertex in G.

Case I. If $v_0 \neq u, v$, without loss of the generality, we may assume that $v_0 = x_i$. We show that $i(G') \leqslant i(G_1)$ in the following, where G_1 is one of graphs showed in figure 6(c) and (d).

If $l > 2$, we may assume $i > 1$.

Let $G'' = (G' - \{x_{i-1}x_{i-2}\}) + \{x_i x_{i-2}\}$. We can show that $i(G') < i(G'')$ by constructing an injective, non-surjective mapping ρ from $I(G')$ to $I(G'')$ as in table 1. The mapping ρ is injective. However, there is no $B \in I(G')$ with $\rho(B) = \{x_{i-1}, x_{i-2}\}$.

We continue this until $l = 2$.

If $l = 2$, then $v_0 = x_1$ and v_0 is adjacent to u and v in G'. We show that $i(G') \leqslant i(G_1)$ in the following:

(i) If $t > 1$, let $G'' = (G' - \{vz_t, z_t z_{t-1}\}) + \{vz_{t-1}, v_0 z_t\})$. Then

$$\begin{aligned}
&i(G'') - i(G') \\
&\quad = i(G'' - \{v_0\}) + i(G'' - N_{G''}[v_0]) \\
&\qquad - i(G' - \{v_0\}) - i(G' - N_{G'}[v_0]) \\
&\quad = 2^{n+4-p-q} i(C_{r+t+1}) + i(P_r \cup P_{t-1}) - 2^{n+3-p-q} i(C_{r+t+2}) - i(P_r \cup P_t) \\
&\quad = 2^{n+4-p-q}(f(r+t) + f(r+t+2)) + f(r+2)f(t+1) \\
&\qquad - 2^{n+3-p-q}(f(r+t+1) + f(r+t+3)) - f(r+2)f(t+2) \\
&\quad = 2^{n+3-p-q}(f(r+t) + f(r+t+2) - f(r+t-1)) - f(r+2)f(t) \\
&\quad = 2^{n+3-p-q}(f(r+t-2) + f(r+t+2)) - f(r+2)f(t) \\
&\quad > 0
\end{aligned}$$

since $f(r+t-2) + f(r+t+2) > f(r+t-1) + f(r+t+1) = i(C_{r+t})$ and $f(r+2)f(t) = i(P_r \cup P_{t-2})$, and there are two vertices v_1, v_2 such that $C_{r+t} - \{v_1, v_2\} = P_r \cup P_{t-2}$, so $f(r+t) + f(r+t+2) > f(r+2)f(t)$. And $i(G') < i(G'')$.

Table 2
The mapping $\xi : I(G') \to I(G'')$.

u	y_1	y_2	ξ
0	0	0	B
0	0	1	B
0	1	0	B
1	0	0	B
1	0	1	$(B - \{u\}) \cup \{y_1\}$

(ii) Similarly, if $r > 1$, let $G'' = (G' - \{vy_r, y_r y_{r-1}\}) + \{vy_{r-1}, v_0 y_r\})$, then also $i(G') < i(G'')$.

Repeating (i) and (ii), we have $i(G') < i(G_1)$.

Case II. If $v_0 = u$ or v, without loss of the generality, we may assume that $v_0 = u$. We show that $i(G') \leqslant i(G_2)$ in the following, where G_2 is the graph showed in figure 6(e).

If $G' \ncong G_2$, then $\{r, t, l-1\} \neq \{1, 2, 2\}$. Without loss of the generality, we may assume that $r \geqslant t \geqslant l-1$ and $r \geqslant 3$. Let $G'' = (G' - \{y_1, y_2\}) + \{uy_2\}$.

We construct a mapping ξ from $I(G')$ to $I(G'')$ as in table 2. The mapping ξ is injective. However, there is no $B \in I(G')$ with $\xi(B) = \{y_1, y_2\}$. So, $i(G') < i(G'')$.

And continuing, we can get $i(G') < i(G_2)$.

6. Extremal graph in $\mathcal{G}(n, n+1)$

In this section, we give the upper bound for the Merrifield–Simmons index in $\mathcal{G}(n, n+1)$, and characterize the extremal graph.

Theorem 6.1. Let G be an $(n, n+1)-$graph, then $i(G) \leqslant 5 \times 2^{n-4} + 1$ with the equality if and only if G is the graph in figure 6(e).

Proof. From theorems 3.4, 4.9, and 5.1, we only need to compare the Merrifield–Simmons indices of $S_n(3,3)$, $T_n^1(3,3)$ and H_1, H_2, H_3, where H_1, H_2, and H_3 are the graphs in figure 6(c),(d), and (e), respectively. Computing immediately, we have

$$i(S_n(3,3)) = 9 \times 2^{n-5} + 1$$

$$i(T_n^1(3,3)) = 12 \times 2^{n-6} + 3 = 6 \times 2^{n-5} + 3$$

$$i(H_1) = 7 \times 2^{n-5} + 4$$

$$i(H_2) = 4 \times 2^{n-4} + 2 = 8 \times 2^{n-5} + 2$$

$$i(H_3) = 5 \times 2^{n-4} + 1 = 10 \times 2^{n-5} + 1$$

Therefore, $i(G) \leqslant i(H_3) = 5 \times 2^{n-4} + 1$ with the equality if and only if G is the graph in figure 6(e).

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