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The Smallest Hosoya Index of Bicyclic Graphs with Given Pendent Vertices

Lihua YOU[1,*], Chaoxia WEI[1], Zhifu YOU[2]
1. *School of Mathematical Sciences, South China Normal University, Guangdong* 510631*, P. R. China;*
2. *School of Computer Science, Guangdong Polytechnic Normal University, Guangdong* 510665*, P. R. China*

Abstract Let G be a graph. The Hosoya index $Z(G)$ of a graph G is defined to be the total number of its matchings. In this paper, we characterize the graph with the smallest Hosoya index of bicyclic graphs with given pendent vertices. Finally, we present a new proof about the smallest Hosoya index of bicyclic graphs.

Keywords Hosoya index; bicyclic graph; pendent vertex; matching.

MR(2010) Subject Classification 05C35; 05C70; 92E10

1. Introduction

The Hosoya index of G, denoted by $Z(G)$, is defined to be the total number of its matchings (independent edge subsets), namely, $Z(G)=\sum_{s=0}^{\lfloor \frac{n}{2}\rfloor} m(G,s)$, where $m(G,s)$ denotes the number of s-matchings of G, and $m(G,0)=1$. It was introduced by Hosoya in 1971 (see [1]), and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures.

Many results have been obtained on the Hosoya index of graphs, for example, a survey [2], trees [3–7], quasi-tree graphs [8], unicyclic graphs [9–12], bicyclic graphs [13], cacti [14]. In [2], Wanger and Gutman pointed out that since the aforementioned questions can be answered for trees with fixed diameter [3], trees with given pendent vertices [5, 7], unicyclic graphs with given pendent vertices [10], and graphs with given clique number [15], it is also natural to consider the analogous questions for other treelike graphs.

In this paper we investigate the bicyclic graphs with given pendent vertices, and characterize the graph with the smallest Hosoya index of bicyclic graphs with given pendent vertices. Moreover, we present a new proof of the result in [13].

2. Some preliminaries

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* Corresponding author
E-mail address: ylhua@scnu.edu.cn (Lihua YOU); 970535930@qq.com (Chaoxia WEI); youzhf@hotmail.com (Zhifu YOU)

In this section, we introduce some definitions, notations and basic properties which we need to use in the proofs of our main results. Other undefined notations may refer to [16].

Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. For any $v \in V$, $N_G(v) = \{u|uv \in E\}$ denotes the neighbors of v, and $d_G(v) = |N_G(v)|$ is the degree of v in G. A pendent vertex is a vertex of degree one. For $E' \subseteq E$ and $V' \subseteq V$, we denote by $G - E'$ and $G - V'$, the subgraphs of G obtained by deleting the edges of E', the vertices of V' and the edges incident with them, respectively.

Let P_n be the path on n vertices, C_n be the cycle on n vertices, and S_n be the star on n vertices. Let T_n^k be a tree with n vertices and k pendent vertices, and S_n^k be a tree obtained from a star S_{k+1} by attaching a path P_{n-k} to a pendent vertex of S_{k+1}.

The following basic results will be used and can be found in the references cited.

Lemma 2.1 *(1) If $e = uv$ is an edge of a graph G, then $Z(G) = Z(G - e) + Z(G - \{u, v\})$.*

(2) If v is a vertex of a graph G, then $Z(G) = Z(G - v) + \sum_{u \in N_G(v)} Z(G - \{v, u\})$.

(3) If G is a graph with components $G_1, G_2, \ldots, G_t$, then $Z(G) = \Pi_{i=1}^{t} Z(G_i)$.

(4) For paths, stars and cycles, we have $Z(P_1) = 1, Z(P_n) = F_{n+1}$ for $n \geq 2$, $Z(S_n) = n, Z(C_n) = F_{n-1} + F_{n+1}$, where F_n denotes the n-th Fibonacci number such that $F_0 = 0, F_1 = 1$ and $F_n = F_{n-1} + F_{n-2}$ for $n \geq 2$, $F_n = F_k F_{n-k+1} + F_{k-1} F_{n-k}$ for $1 \leq k \leq n$.

For convenience, let $Z(P_0) = 1$. Thus $Z(P_n) = F_{n+1}$ for $n \geq 0$.

Transformation A ([14]) Let H, X, Y be three connected disjoint graphs. Suppose that u, v are two vertices of H, u_1 is a vertex of X, v_1 is a vertex of Y. Let G^* be the graph resulting from H, X, Y by identifying u with u_1, and v with v_1, respectively. Let G_u^* be the graph obtained from H, X, Y by identifying vertices u, u_1, v_1, and G_v^* be the graph obtained from H, X, Y by identifying vertices v, u_1, v_1 (see Figure 1).

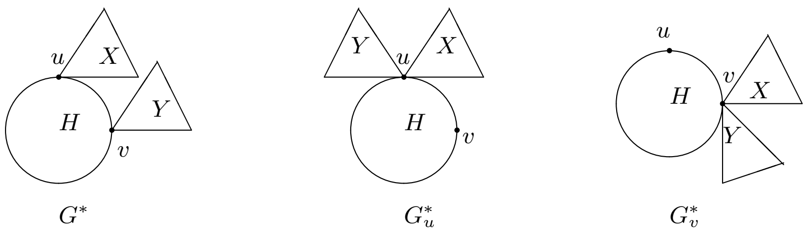


Figure 1 Graphs G^*, G_u^*, G_v^* from H, X, Y by Transformation A

Lemma 2.2 ([14]) *Let G^*, G_u^*, G_v^* be graphs obtained from H, X, Y by Transformation A. Then $Z(G^*) \geq Z(G_u^*)$ or $Z(G^*) \geq Z(G_v^*)$.*

Transformation B ([6]) Let t, n be integers with $1 \leq t \leq n$, H be a connected graph. Choose $v \in V(H)$. Let $P(n, t, H, v)$ (see Figure 2) be the graph resulting from H and a path $P_n = v_1 v_2 \cdots v_t \cdots v_n$ by identifying v with the vertex v_t.

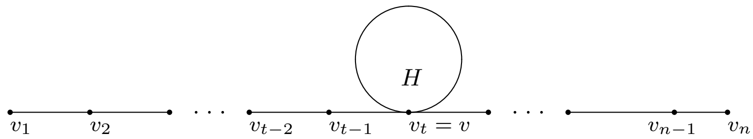


Figure 2 Graph $P(n,t,H,v)$ from H and P_n by Transformation B

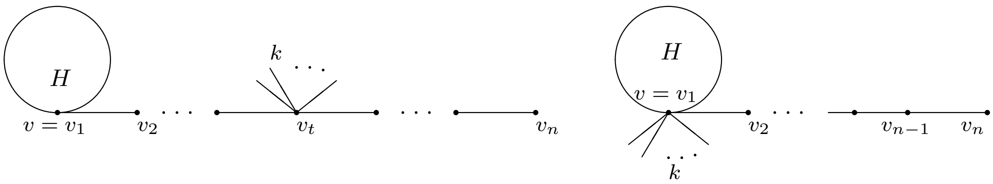
Lemma 2.3 ([6]) *Let t,n,l,m,i be integers with $1 \le t \le n = 4m+i$ where $m \ge 0$, $i \in \{1,2,3,4\}$, $l = \lfloor \frac{i-1}{2} \rfloor$, H be a connected graph but not a path and $v \in V(H)$, $P(n,t,H,v)$ be the graph obtained from H and P_n by Transformation B. Then*

$$\begin{aligned} &Z(P(n,2,H,v)) < Z(P(n,4,H,v)) < \cdots < Z(P(n,2m+2l,H,v)) \\ &\quad < Z(P(n,2m+1,H,v)) < \cdots < Z(P(n,3,H,v)) < Z(P(n,1,H,v)). \end{aligned}$$

Lemma 2.4 *Let t,n,k be nonnegative integers with $1 \le t \le n-1$, H be a connected graph but not a path and $v \in V(H)$, $P(n,1,H,v,t,k)$ (see Figure 3) be the graph obtained from H and a path $P_n = v_1 v_2 \cdots v_t \cdots v_n$ by identifying v with the vertex v_1, and adding k pendent edges to $v_t \in V(P_n)$. Then we have*

(1) $Z(P(n,1,H,v,1,k)) = Z(H)F_n + Z(H-v)F_{n-1} + kZ(H-v)F_n$.

(2) If $t \ge 2$, then $Z(P(n,1,H,v,t,k)) = Z(H)F_n + Z(H-v)F_{n-1} + k(Z(H-v)F_{t-2} + Z(H)F_{t-1})F_{n-t+1}$.



Graph $P(n,1,H,v,t,k)$ for $t \ge 2$ Graph $P(n,1,H,v,1,k)$

Figure 3 Graph $P(n,1,H,v,t,k)$

Proof We only prove (2) since the proof of (1) is similar.

Case 1 $k = 0$.

Note that $P(n,1,H,v,t,0) = P(n,1,H,v)$, and let $e = v_1 v_2$. By (1), (3), (4) of Lemma 2.1, we have $Z(P(n,1,H,v)) = Z(H)Z(P_{n-1}) + Z(H-v)Z(P_{n-2}) = Z(H)F_n + Z(H-v)F_{n-1}$.

Case 2 $k \ge 1$.

Let e be one of the k pendent edges added to v_t. By (1), (3), (4) of Lemma 2.1, we have

$$\begin{aligned} Z(P(n,1,H,v,t,k)) &= Z(P(n,1,H,v,t,k-1)) + Z(P(t-1,1,H,v))Z(P_{n-t}) \\ &= Z(P(n,1,H,v,t,k-2)) + 2Z(P(t-1,1,H,v))Z(P_{n-t}) \\ &= \cdots \\ &= Z(P(n,1,H,v,t,0)) + kZ(P(t-1,1,H,v))Z(P_{n-t}). \end{aligned}$$

Case 2.1 $t = 2$. It is clear.

Case 2.2 $t \geq 3$.

$$\begin{aligned}Z(P(n,1,H,v,t,k)) =& Z(H)Z(P_{n-1}) + Z(H-v)Z(P_{n-2}) + \\ & k[Z(H)Z(P_{t-2}) + Z(H-v)Z(P_{t-3})]Z(P_{n-t}) \\ =& Z(H)F_n + Z(H-v)F_{n-1} + k(Z(H-v)F_{t-2} + Z(H)F_{t-1})F_{n-t+1}.\end{aligned}$$

Hence (2) follows.

Remark 2.5 In Lemma 2.4, if H is a cycle on r vertices and $k=0$, we have

$$\begin{aligned}Z(P(n,1,C_r,v,t,0)) =& Z(P(n,1,C_r,v)) \\ =& Z(C_r)Z(P_{n-1}) + Z(C_r - v)Z(P_{n-2}) \\ =& 2F_{r-1}F_n + F_rF_{n+1}.\end{aligned}$$

For nonnegative integers $n, r(\geq 3)$, let $f(n,r) = 2F_{r-1}F_n + F_rF_{n+1}$. Then $f(n,r) = Z(P(n,1,C_r,v))$ for $n \geq 1$. Note that $f(0,r) = F_r = Z(P_{r-1})$, for convenience, we can define $f(0,r) = Z(P(0,1,C_r,v))$. Therefore, $f(n,r) = Z(P(n,1,C_r,v))$ for $n \geq 0$.

It is easy to prove the following proposition.

Proposition 2.6 *Let $n, r(\geq 3)$ be positive integers. Then*

(1) $f(n,r) = f(n-1,r) + f(n-2,r)$ *for* $n \geq 2$.

(2) $f(n,r) < 3f(n-1,r)$ *for* $n \geq 1$.

The following Lemmas 2.7–2.10 will play an important role in Sections 3–5.

Lemma 2.7 *Let $n \geq 4$, F_n be the n-th Fibonacci number. Then* $\frac{3}{5} \leq \frac{F_{n-1}}{F_n} \leq \frac{2}{3}$.

Proof By induction on n.

It is obvious that $\frac{F_3}{F_4} = \frac{2}{3}$, $\frac{F_4}{F_5} = \frac{3}{5}$. Then for $n = 4, 5$, the result holds.

Suppose the result holds for $n = s$ $(s \geq 4)$. For $n = s+1$,

$$\frac{8}{5}F_s = F_s + \frac{3}{5}F_s \leq F_{s+1} = F_s + F_{s-1} \leq F_s + \frac{2}{3}F_s = \frac{5}{3}F_s,$$

thus $\frac{3}{5} = \frac{F_s}{\frac{5}{3}F_s} \leq \frac{F_s}{F_{s+1}} = \frac{F_s}{F_s + F_{s-1}} \leq \frac{F_s}{\frac{8}{5}F_s} = \frac{5}{8} < \frac{2}{3}$. The result follows.

Remark 2.8 Note that $\frac{F_2}{F_3} = \frac{1}{2} < \frac{2}{3}$, then $\frac{F_{n-1}}{F_n} \leq \frac{2}{3}$ holds for all $n \geq 3$.

Lemma 2.9 *Let $n(\geq 3), t, k$ be positive integers with $1 \leq t \leq n-1$, and $P(n,1,H,v,t,k)$ be defined as before. If $Z(H-v) < \frac{3}{2}\sum_{u \in N_H(v)} Z(H - \{v,u\})$, then*

$$Z(P(n,1,H,v,1,k)) \leq Z(P(n,1,H,v,t,k)),$$

with the equality holding if and only if $t = 1$.

Proof We only need to show $Z(P(n,1,H,v,1,k)) < Z(P(n,1,H,v,t,k))$ when $t \geq 2$.

Suppose $t \geq 2$, by Lemmas 2.4, 2.7, and (2), (4) of Lemma 2.1, we have

$Z(P(n,1,H,v,1,k)) - Z(P(n,1,H,v,t,k))$

$$= kZ(H-v)F_n - kZ(H-v)F_{t-2}F_{n-t+1} - kZ(H)F_{t-1}F_{n-t+1}$$
$$= kZ(H-v)F_n - kZ(H-v)F_{t-2}F_{n-t+1} - k(Z(H-v) + \sum_{u\in N_H(v)} Z(H-\{v,u\}))F_{t-1}F_{n-t+1}$$
$$= kZ(H-v)[F_n - (F_{t-2}+F_{t-1})F_{n-t+1}] - k\sum_{u\in N_H(v)} Z(H-\{v,u\})F_{t-1}F_{n-t+1}$$
$$= kZ(H-v)(F_n - F_tF_{n-t+1}) - k\sum_{u\in N_H(v)} Z(H-\{v,u\})F_{t-1}F_{n-t+1}$$
$$= kZ(H-v)F_{t-1}F_{n-t} - k\sum_{u\in N_H(v)} Z(H-\{v,u\})F_{t-1}F_{n-t+1}$$
$$= kF_{t-1}[Z(H-v)F_{n-t} - \sum_{u\in N_H(v)} Z(H-\{v,u\})F_{n-t+1}]$$
$$\le kF_{t-1}F_{n-t}[Z(H-v) - \frac{3}{2}\sum_{u\in N_H(v)} Z(H-\{v,u\})].$$

Then $Z(P(n,1,H,v,1,k)) < Z(P(n,1,H,v,t,k))$ by $Z(H-v) < \frac{3}{2}\sum_{u\in N_G(v)} Z(H-\{v,u\})$. The result holds. □

Lemma 2.10 *Let n,k be nonnegative integers, H be a connected graph and $x \in V(H)$, $P(n,1,H,x,1,k)$ be defined as above. If $Z(H-u) < Z(H-v)$ for $u,v \in V(H)$, then we have $Z(P(n,1,H,u,1,k)) < Z(P(n,1,H,v,1,k))$.*

Proof By (1) of Lemma 2.4,

$$Z(P(n,1,H,u,1,k)) - Z(P(n,1,H,v,1,k)) = [Z(H-u) - Z(H-v)][kF_n + F_{n-1}] < 0. \quad \square$$

Let $\mathcal{G}(n,n+1,k)$ be the set of bicyclic graphs on n vertices and k pendent vertices. For any graph $G \in \mathcal{G}(n,n+1,k)$, there are two cycles of C_p, C_q and k pendent vertices in G.

Let $G^0(p,q,k)$ be the set of $G \in \mathcal{G}(n,n+1,k)$ in which the cycles C_p and C_q do not have common vertices, and $G^l(p,q,k)(l \ge 1)$ be the set of $G \in \mathcal{G}(n,n+1,k)$ in which the cycles C_p and C_q have l common vertices. Let $G(0,k)$ be the set of $G \in \mathcal{G}(n,n+1,k)$ in which the two cycles do not have common vertices, and $G(l,k)(l \ge 1)$ be the set of $G \in \mathcal{G}(n,n+1,k)$ in which the two cycles have l common vertices. Clearly, $G^0(p,q,k) \subseteq G(0,k)$ and $G^l(p,q,k) \subseteq G(l,k)$ for $l \ge 1$.

In Sections 3–5, we will characterize the graph on n vertices with the smallest Hosoya index in $G(0,k)$, $G(1,k)$, and $G(l,k)$ $(l \ge 2)$, respectively.

3. The graph with the smallest Hosoya index in $G(0,k)$

In this section, we will characterize the graph on n vertices with the smallest Hosoya index in $G(0,k)$.

Let $s, p(\ge 3), q(\ge 3), l(\ge 2)$ be positive integers with $s = p+q+l-2$, $S_l(p,q)$ be the graph on s vertices, obtained by connecting C_p and C_q by a path P_l (see Figure 4). For convenience, we let $u_1(u_4)$ be the common vertex of P_l and $C_p(C_q)$, $u_2 \in V(C_p)\backslash\{u_1\}$, $u_3 \in V(P_l)\backslash\{u_1,u_4\}$

(if $l \geq 3$), $u_5 \in V(C_q)\backslash\{u_4\}$.

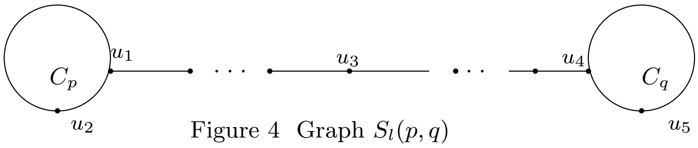


Figure 4 Graph $S_l(p, q)$

Lemma 3.1 *For* $1 \leq i \leq 5$, *we have* $Z(S_l(p,q) - u_i) < \frac{3}{2}\sum_{x \in N_{S_l(p,q)}(u_i)} Z(S_l(p,q) - \{x, u_i\})$.

Proof There are five cases.

Case 1 $i = 1$.

By Lemma 2.1, Remark 2.5 and $F_p \leq 2F_{p-1}$,

$$\begin{aligned}
&Z(S_l(p,q) - u_1) - \frac{3}{2}\sum_{x \in N_{S_l(p,q)}(u_1)} Z(S_l(p,q) - \{x, u_1\}) \\
&< Z(S_l(p,q) - u_1) - \sum_{x \in N_{S_l(p,q)}(u_1)} Z(S_l(p,q) - \{x, u_1\}) \\
&= Z(P(l-1, 1, C_q, u_4))Z(P_{p-1}) - \\
&\quad [2Z(P_{p-2})Z(P(l-1, 1, C_q, u_4)) + Z(P_{p-1})Z(P(l-2, 1, C_q, u_4))] \\
&= f(l-1, q)(F_p - 2F_{p-1}) - f(l-2, q)F_p < 0.
\end{aligned}$$

Case 2 $i = 2$.

Let $d(u_1, u_2) = t - 1$, $u_1^*(\in P_l)$ be adjacent to u_1 and $e = u_1u_1^*$. Then $t \geq 2$. By Lemma 2.1, Remark 2.5 and $F_p \leq 2F_{p-1} < 3F_{p-1}$, we have

Subcase 2.1 $t \geq 3$.

$$\begin{aligned}
&2Z(S_l(p,q) - u_2) - 3\sum_{x \in N_{S_l(p,q)}(u_2)} Z(S_l(p,q) - \{x, u_2\}) \\
&= 2(Z(S_l(p,q) - u_2 - e) + Z(S_l(p,q) - \{u_1, u_1^*, u_2\})) - \\
&\quad 3\sum_{x \in N_{S_l(p,q)}(u_2)} [Z(S_l(p,q) - \{x, u_2\} - e) + Z(S_l(p,q) - \{x, u_2, u_1, u_1^*\})] \\
&= 2Z(P(l-1, 1, C_q, u_4))Z(P_{p-1}) + 2Z(P(l-2, 1, C_q, u_4))Z(P_{t-2})Z(P_{p-t}) - \\
&\quad [6Z(P(l-1, 1, C_q, u_4))Z(P_{p-2}) + 3Z(P(l-2, 1, C_q, u_4))(Z(P_{t-3})Z(P_{p-t}) + \\
&\quad Z(P_{t-2})Z(P_{p-t-1}))] \\
&= 2f(l-1, q)(F_p - 3F_{p-1}) + f(l-2, q)[(F_{t-1} - 3F_{t-2})F_{p-t+1} + F_{t-1}(F_{p-t+1} - 3F_{p-t})] < 0.
\end{aligned}$$

Subcase 2.2 $t = 2$.

$$\begin{aligned}
&Z(S_l(p,q) - u_2) - \frac{3}{2}\sum_{x \in N_{S_l(p,q)}(u_2)} Z(S_l(p,q) - \{x, u_2\}) \\
&< Z(S_l(p,q) - u_2) - \sum_{x \in N_{S_l(p,q)}(u_2)} Z(S_l(p,q) - \{x, u_2\}) \\
&= (Z(S_l(p,q) - u_2 - e) + Z(S_l(p,q) - \{u_1, u_1^*, u_2\})) -
\end{aligned}$$

$$\sum_{x\in N_{S_l(p,q)}(u_2)} [Z(S_l(p,q)-\{x,u_2\}-e)+Z(S_l(p,q)-\{x,u_2,u_1,u_1^*\})]$$
$$=Z(P(l-1,1,C_q,u_4))Z(P_{p-1})+Z(P(l-2,1,C_q,u_4))Z(P_{p-2})-$$
$$[2Z(P(l-1,1,C_q,u_4))Z(P_{p-2})+Z(P(l-2,1,C_q,u_4))(Z(P_{p-2})+Z(P_{p-3}))]$$
$$=f(l-1,q)(F_p-2F_{p-1})-f(l-2,q)F_{p-2}<0.$$

Case 3 $i=3$.

Let $d(u_1,u_3)=h_1-1$. Then $h_1\geq 2$ and $l\geq h_1+1\geq 3$. By Lemma 2.1, Remark 2.5 and Proposition 2.6, we have

$$2Z(S_l(p,q)-u_3)-3\sum_{x\in N_{S_l(p,q)}(u_3)} Z(S_l(p,q)-\{x,u_3\})$$
$$=2Z(P(h_1-1,1,C_p,u_1))Z(P(l-h_1,1,C_q,u_4))-$$
$$3Z(P(h_1-2,1,C_p,u_1))Z(P(l-h_1,1,C_q,u_4))-$$
$$3Z(P(h_1-1,1,C_p,u_1))Z(P(l-h_1-1,1,C_q,u_4))$$
$$=(f(h_1-1,p)-3f(h_1-2,p))f(l-h_1,q)+f(h_1-1,p)(f(l-h_1,q)-3f(l-h_1-1,q))<0.$$

Case 4 $i=4$. It is similar to Case 1.

Case 5 $i=5$. It is similar to Case 2.

Combining the above arguments, we prove the result.

By Lemmas 2.9 and 3.1, we have

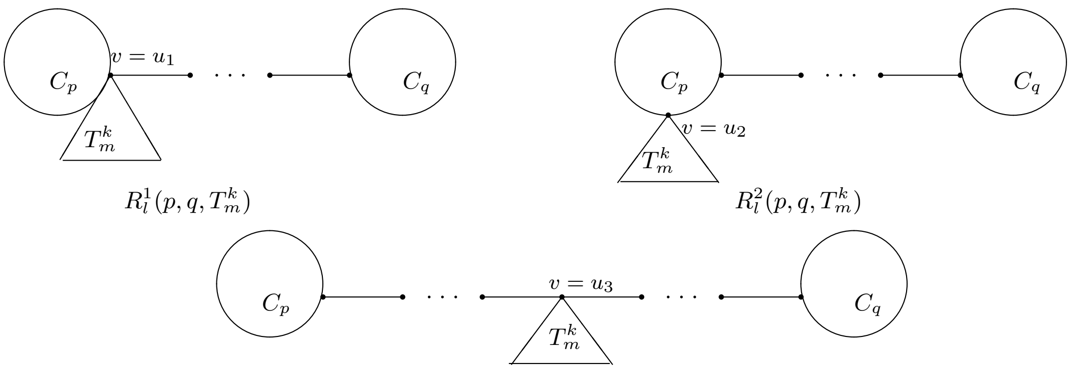
Corollary 3.2 *Let $n(\geq 3),t,k$ be positive integers with $1\leq t\leq n-1$, $P(n,1,H,v,t,k)$ and $S_l(p,q)$ be defined as before. Then for any $i(1\leq i\leq 5)$,*

$$Z(P(n,1,S_l(p,q),u_i,1,k))\leq Z(P(n,1,S_l(p,q),u_i,t,k))$$

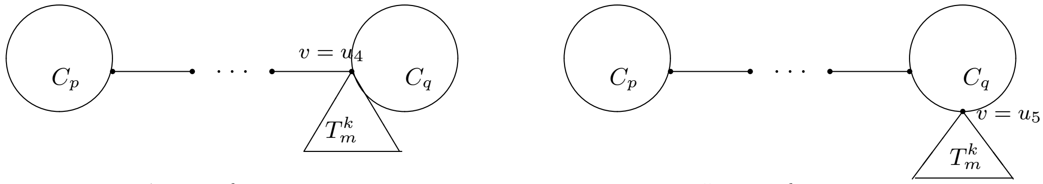
with the equality holding if and only if $t=1$.

Let G_1 and G_2 be two graphs, $v_1\in V(G_1)$, $v_2\in V(G_2)$. $G=(G_1,v_1)\triangle(G_2,v_2)$ denotes the graph resulting from identifying v_1 with v_2 as one common vertex.

Let m,k be positive integers with $2\leq k\leq m-1$, $v\in V(T_m^k)$ and $d(v)\geq 2$. Take $R_l^i(p,q,T_m^k)=(S_l(p,q),u_i)\triangle(T_m^k,v)$ $(i=1,2,3,4,5)$ (see Figure 5), then $R_l^i(p,q,T_m^k)\in G^0(p,q,k)$.



$R_l^3(p,q,T_m^k)$



$R_l^4(p, q, T_m^k)$ $R_l^5(p, q, T_m^k)$

Figure 5 $R_l^i(p, q, T_m^k)$ $(i = 1, 2, 3, 4, 5)$

Lemma 3.3 *Let m, k, p, q, l, t be positive integers with $p, q \geq 3$, $l \geq 2$ and $2 \leq k \leq m - 1$, $S_l(p, q)$, u_i, $R_l^i(p, q, T_m^k)$, $P(m - k + 1, 1, S_l(p, q), u_i, t, k - 1)$ be defined as before for $1 \leq i \leq 5$. Then for any $i(1 \leq i \leq 5)$, there exists some integer t with $1 \leq t \leq m - k$ such that*

$$Z(R_l^i(p, q, T_m^k)) \geq Z(P(m - k + 1, 1, S_l(p, q), u_i, t, k - 1)).$$

Proof For any $i(1 \leq i \leq 5)$, repeating Transformations A and B on $R_l^i(p, q, T_m^k)$, we get a graph $P(m - k + 1, 1, S_l(p, q), u_i, t, k - 1)$. By Lemmas 2.2 and 2.3, $Z(R_l^i(p, q, T_m^k)) \geq Z(P(m - k + 1, 1, S_l(p, q), u_i, t, k - 1))$.

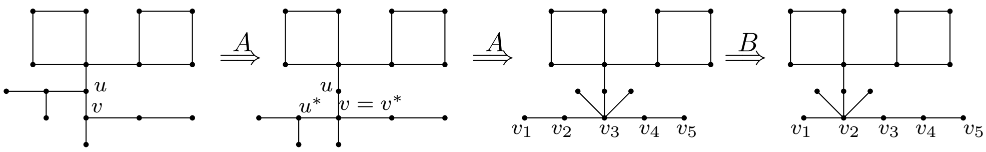


Figure 6 $R_2^1(4, 4, T_9^4)$ is transformed to $Z(P(6, 1, S_2(4, 4), u_1, 3, 3))$ by Transformations A and B

Note that $R_l^i(p, q, S_m^k) = P(m - k + 1, 1, S_l(p, q), u_i, 1, k - 1)$, by Corollary 3.2 and Lemma 3.3, we can get the following corollary immediately.

Corollary 3.4 *Let $1 \leq i \leq 5$. We have $Z(R_l^i(p, q, T_m^k)) \geq Z(R_l^i(p, q, S_m^k))$, with the equality holding if and only if $T_m^k = S_m^k$.*

Lemma 3.5 *Suppose $G \in G^0(p, q, k)$ on n vertices, and P_l is the path connecting C_p and C_q with length $l - 1$. Then $Z(G) \geq Z(R_l^1(p, q, S_m^k))$ or $Z(G) \geq Z(R_l^4(p, q, S_m^k))$.*

Proof It is obvious that there exists some i $(1 \leq i \leq 5)$ and some tree T_m^k such that $Z(G) \geq Z(R_l^i(p, q, T_m^k))$ by Transformation A. Then we only need to show $Z(R_l^i(p, q, S_m^k)) > Z(R_l^1(p, q, S_m^k))$ for $i = 2, 3$ and $Z(R_l^j(p, q, S_m^k)) > Z(R_l^4(p, q, S_m^k))$ for $j = 3, 5$ by Corollary 3.4.

Note that $R_l^i(p, q, S_m^k) = P(m - k + 1, 1, S_l(p, q), u_i, 1, k - 1)$, we only need to show the following inequalities by Lemma 2.10:

$$Z(S_l(p, q) - u_1) < Z(S_l(p, q) - u_2) \tag{3.1}$$

$$Z(S_l(p, q) - u_1) < Z(S_l(p, q) - u_3) \tag{3.2}$$

$$Z(S_l(p, q) - u_4) < Z(S_l(p, q) - u_5) \tag{3.3}$$

$$Z(S_l(p,q)-u_4)<Z(S_l(p,q)-u_3) \tag{3.4}$$

Now we show (3.1). Let $d(u_1,u_2)=t-1$. Then $t\geq 2$.

Case 1 $t=2$.

$$\begin{aligned}Z(S_l(p,q)-u_1)-Z(S_l(p,q)-u_2)&=f(l-1,q)Z(P_{p-1})-f(l-1,q)Z(P_{p-1})-f(l-2,q)Z(P_{p-2})\\&=-f(l-2,q)Z(P_{p-2})<0.\end{aligned}$$

Case 2 $t\geq 3$.

$$\begin{aligned}&Z(S_l(p,q)-u_1)-Z(S_l(p,q)-u_2)\\&\quad=f(l-1,q)Z(P_{p-1})-f(l-1,q)Z(P_{p-1})-f(l-2,q)Z(P_{p-t})Z(P_{t-2})\\&\quad=-f(l-2,q)Z(P_{p-t})Z(P_{t-2})<0.\end{aligned}$$

Now we show (3.2). Let $d(u_1,u_3)=h_1-1$. Then $h_1\geq 2$ and $l\geq h_1+1\geq 3$.

$$\begin{aligned}&Z(S_l(p,q)-u_1)-Z(S_l(p,q)-u_3)\\&\quad=Z(P_{p-1})f(l-1,q)-f(h_1-1,p)f(l-h_1,q)\\&\quad=F_p(2F_{q-1}F_{l-1}+F_qF_l)-(2F_{p-1}F_{h_1-1}+F_pF_{h_1})(2F_{q-1}F_{l-h_1}+F_qF_{l-h_1+1})\\&\quad=F_{q-1}F_{h_1-1}(F_pF_{l-h_1-1}-2F_{p-1}F_{l-h_1})+F_qF_{h_1-1}(F_pF_{l-h_1}-2F_{p-1}F_{l-h_1+1})\\&\quad<0.\end{aligned}$$

Since the proof of (3.3) (or (3.4)) is similar to that of (3.1) (or (3.2)) by the symmetry of C_p and C_q, we ignore it. The result follows.

Lemma 3.6 *Let l,m,k,p,q be positive integers with $l\geq 2$, $p,q\geq 3$ and $2\leq k\leq m-1$, $R_l^1(p,q,T_m^k)$ and u_i $(1\leq i\leq 5)$ be defined as above. Then*

$$Z(R_l^1(p,q,S_m^k))=[kF_pF_{m-k+1}+F_pF_{m-k}+2F_{p-1}F_{m-k+1}]f(l-1,q)+F_pF_{m-k+1}f(l-2,q).$$

Proof By Lemma 2.1,

$$\begin{aligned}Z(R_l^1(p,q,S_m^k))&=Z(R_l^1(p,q,S_m^k)-u_1)+\sum_{x\in N_{R_l^1(p,q,S_m^k)}(u_1)}Z(R_l^1(p,q,S_m^k)-\{u_1,x\})\\&=Z(P(l-1,1,C_q,u_4))Z(P_{p-1})Z(P_{m-k})+\sum_{x\in N_{S_l(p,q)}(u_1)}Z(S_l(p,q)-\{u_1,x\})Z(P_{m-k})+\\&\quad\sum_{x\in N_{S_m^k}(u_1)}Z(S_m^k-\{u_1,x\})Z(P(l-1,1,C_q,u_4))Z(P_{p-1})\\&=[kF_pF_{m-k+1}+F_pF_{m-k}+2F_{p-1}F_{m-k+1}]f(l-1,q)+F_pF_{m-k+1}f(l-2,q).\end{aligned}$$

Lemma 3.7 *Let l,m,k,p,q be positive integers with $l\geq 2$, $p,q\geq 3$, $l+q-3\geq 3$ and $2\leq k\leq m-1$. Then $Z(R_l^1(p,q,S_m^k))\geq Z(R_3^1(p,l+q-3,S_m^k))$, with the equality holding if and only if $R_l^1(p,q,S_m^k)\cong R_3^1(p,l+q-3,S_m^k)$.*

Proof There are two cases.

Case 1 $l \geq 3$.

Firstly, by Remark 2.5, we have

$$\begin{aligned}f(2,l+q-3)-f(l-1,q) =&(2F_{l+q-4}F_2+F_{l+q-3}F_3)-(2F_{q-1}F_{l-1}+F_qF_l)\\ =&2F_{l+q-2}-2F_{q-1}F_{l-1}-F_qF_l\\ =&2F_{l-1}F_q+2F_{l-2}F_{q-1}-2F_{q-1}F_{l-1}-F_qF_l\\ =&(2F_{l-1}-F_l)F_q+2F_{q-1}(F_{l-2}-F_{l-1})\\ =&-F_{l-3}F_{q-3}\leq 0.\\ f(1,l+q-3)-f(l-2,q) =&(2F_{l+q-4}F_1+F_{l+q-3}F_2)-(2F_{q-1}F_{l-2}+F_qF_{l-1})\\ =&F_{l+q-4}+F_{l+q-2}-2F_{q-1}F_{l-2}-F_qF_{l-1}\\ =&(F_{l-1}F_{q-2}+F_{l-2}F_{q-3})+(F_{l-1}F_q+F_{l-2}F_{q-1})-\\ &2F_{q-1}F_{l-2}-F_qF_{l-1}\\ =&F_{l-1}F_{q-2}+F_{l-2}(F_{q-3}-F_{q-1})\\ =&F_{l-3}F_{q-2}\geq 0.\end{aligned}$$

Then by Lemma 3.6 and $F_{q-2}-kF_{q-3}\leq 0$ for $k\geq 2$,

$$\begin{aligned}&Z(R_3^1(p,l+q-3,S_m^k))-Z(R_l^1(p,q,S_m^k))\\ &=[kF_pF_{m-k+1}+F_pF_{m-k}+2F_{p-1}F_{m-k+1}][f(2,l+q-3)-f(l-1,q)]+\\ &\quad F_pF_{m-k+1}[f(1,l+q-3)-f(l-2,q)]\\ &=[kF_pF_{m-k+1}+F_pF_{m-k}+2F_{p-1}F_{m-k+1}][-F_{l-3}F_{q-3}]+\\ &\quad F_pF_{m-k+1}F_{l-3}F_{q-2}\\ &=[F_{q-2}-kF_{q-3}]F_pF_{m-k+1}F_{l-3}-[F_pF_{m-k}+2F_{p-1}F_{m-k+1}]F_{l-3}F_{q-3}\leq 0.\end{aligned}$$

It is obvious that the equality holds if and only if $l=3$. □

Case 2 $l=2$.

Note that $q\geq 4$ by $l+p-3\geq 3$. Then by Lemma 3.6 and $F_{q-2}-kF_{q-3}\leq 0$ for $k\geq 2$,

$$\begin{aligned}&Z(R_3^1(p,q-1,S_m^k))-Z(R_2^1(p,q,S_m^k))\\ &=[kF_pF_{m-k+1}+F_pF_{m-k}+2F_{p-1}F_{m-k+1}][f(2,q-1)-f(1,q)]+F_pF_{m-k+1}[f(1,q-1)-f(0,q)]\\ &=[kF_pF_{m-k+1}+F_pF_{m-k}+2F_{p-1}F_{m-k+1}][-F_{q-3}]+F_pF_{m-k+1}F_{q-2}\\ &=[F_{q-2}-kF_{q-3}]F_pF_{m-k+1}-[F_pF_{m-k}+2F_{p-1}F_{m-k+1}]F_{q-3}<0.\end{aligned}$$

Lemma 3.8 *Let l,m,k,p,q be positive integers with $l\geq 2$, $p,q\geq 3$ and $2\leq k\leq m-1$. Then $Z(R_l^1(p,q,S_m^k))\geq Z(R_l^1(p+m-k-1,q,S_{k+1}^k))$, with the equality holding if and only if $m=k+1$.*

Proof By $F_n=F_kF_{n-k+1}+F_{k-1}F_{n-k}$,

$$F_pF_{m-k+1}-F_{p+m-k-1}=F_pF_{m-k+1}-(F_{p-1}F_{m-k+1}+F_{p-2}F_{m-k})=F_{p-2}F_{m-k-1}. \quad (3.5)$$

$$F_{p-1}F_{m-k+1} - F_{p+m-k-2} = F_{p-3}F_{m-k-1}. \tag{3.6}$$

$$F_pF_{m-k} - F_{p+m-k-1} = F_pF_{m-k} - (F_pF_{m-k} + F_{p-1}F_{m-k-1}) = -F_{p-1}F_{m-k-1}. \tag{3.7}$$

Then by Lemma 3.6 and (3.5), (3.6), (3.7),

$$\begin{aligned}
&Z(R_l^1(p,q,S_m^k)) - Z(R_l^1(p+m-k-1,q,S_{k+1}^k)) \\
&= [k(F_pF_{m-k+1} - F_{p+m-k-1}) + (F_pF_{m-k} - F_{p+m-k-1})+ \\
&\quad 2(F_{p-1}F_{m-k+1} - F_{p+m-k-2})]f(l-1,q) + (F_pF_{m-k+1} - F_{p+m-k-1})f(l-2,q) \\
&= (kF_{p-2}F_{m-k-1} - F_{p-1}F_{m-k-1} + 2F_{p-3}F_{m-k-1})f(l-1,q) + F_{p-2}F_{m-k-1}f(l-2,q) \\
&= [(k-1)F_{p-2} + F_{p-3}]F_{m-k-1}f(l-1,q) + F_{p-2}F_{m-k-1}f(l-2,q) \geq 0.
\end{aligned}$$

It is obvious that the equality holds if and only if $m = k+1$. □

Lemma 3.9 *Let m,k,p,q be positive integers with $p,q \geq 3$ and $2 \leq k \leq m-1$. Then $Z(R_3^1(p,q,S_{k+1}^k)) \geq Z(R_3^1(p+q-3,3,S_{k+1}^k))$, with the equality holding if and only if $q = 3$.*

Proof Suppose $q > 3$. By $F_n = F_kF_{n-k+1} + F_{k-1}F_{n-k}$,

$$\begin{aligned}
&(F_pF_{q-1} + F_pF_q) - 3F_{p+q-3} \\
&\quad = (F_{p-1}F_{q-1} + F_{p-2}F_{q-1}) + (F_{p-1}F_q + F_{p-2}F_q) - 3(F_{p-1}F_{q-1} + F_{p-2}F_{q-2}) \\
&\quad = (F_{p-2}F_{q-1} - F_{p-2}F_{q-2}) + (F_{p-1}F_q - 2F_{p-1}F_{q-1}) + (F_{p-2}F_q - 2F_{p-2}F_{q-2}) \\
&\quad = (2F_{p-2} - F_{p-1})F_{q-3} \geq 0, \\
&(F_{p-1}F_{q-1} + F_{p-1}F_q) - 3F_{p+q-4} = (2F_{p-3} - F_{p-2})F_{q-3},
\end{aligned}$$

and

$$\begin{aligned}
&F_p(F_{q-1} + F_{q+1}) - 4F_{p+q-3} = 3F_pF_{q-1} + F_pF_{q-2} - 4F_{p+q-3} \\
&\quad = 3(F_{p-1}F_{q-1} + F_{p-2}F_{q-1}) + (F_{p-1}F_{q-2} + F_{p-2}F_{q-2}) - 4(F_{p-1}F_{q-1} + F_{p-2}F_{q-2}) \\
&\quad = (3F_{p-2} - F_{p-1})F_{q-3} > 0.
\end{aligned}$$

Then by Lemma 3.6,

$$\begin{aligned}
&Z(R_3^1(p,q,S_{k+1}^k)) - Z(R_3^1(p+q-3,3,S_{k+1}^k)) \\
&= [(k+1)F_p + 2F_{p-1}]f(2,q) + F_pf(1,q) - [(k+1)F_{p+q-3} + 2F_{p+q-4}]f(2,3) - F_{p+q-3}f(1,3) \\
&= 2(k+1)[(F_pF_{q-1} + F_pF_q) - 3F_{p+q-3}] + 4[(F_{p-1}F_{q-1} + F_{p-1}F_q) - 3F_{p+q-4}]+ \\
&\quad [F_p(F_{q-1} + F_{q+1}) - 4F_{p+q-3}] \\
&= 2(k+1)(2F_{p-2} - F_{p-1})F_{q-3} + 4(2F_{p-3} - F_{p-2})F_{q-3} + (3F_{p-2} - F_{p-1})F_{q-3} \\
&= [2kF_{p-2} - (2k-5)F_{p-3}]F_{q-3} > 0.
\end{aligned}$$

Combining the above arguments, we have the following theorem.

Theorem 3.10 *Let n,k be positive integers with $2 \leq k \leq n-6$ and $G \in \mathcal{G}(n,n+1,k)$ be a bicyclic graph on n vertices and k pendent vertices with the two cycles having no common vertices. Then we have*

(1) If $2 \leq k \leq n-7$, then $Z(G) \geq 6kF_{n-k-4} + 10F_{n-k-3} + 2F_{n-k-5}$, with the equality holding if and only if $G \cong R_3^1(n-k-4, 3, S_{k+1}^k)$.

(2) If $k = n-6$, then $Z(G) \geq 8n-28$, with the equality holding if and only if $G \cong R_2^1(3, 3, S_{n-5}^{n-6})$.

Proof Let p, q be positive integers with $p, q \geq 3$ and $G \in G^0(p, q, k)$ on n vertices. Suppose the two cycles in G are connected by a path P_l with $l \geq 2$. Then there exist $i \in \{1, 2, 3, 4, 5\}$ and some tree T_m^k where $2 \leq k \leq m-1$ and $m = n-p-q-l+3$ such that $Z(G) \geq Z(R_l^i(p, q, T_m^k))$ by Transformation A.

Thus by Corollary 3.4 and Lemma 3.5,

$$Z(G) \geq Z(R_l^i(p, q, T_m^k) \geq Z(R_l^i(p, q, S_m^k) \geq \min\{Z(R_l^1(p, q, S_m^k)), Z(R_l^4(p, q, S_m^k)\}.$$

Noticing the similarity of $R_l^1(p, q, S_m^k)$ and $R_l^4(p, q, S_m^k)$, we only need to consider $Z(R_l^1(p, q, S_m^k))$.

Case 1 $l \geq 3$.

By Lemmas 3.7–3.9,

$$\begin{aligned} Z(R_l^1(p, q, S_m^k)) &\geq Z(R_3^1(p, l+q-3, S_m^k)) \geq Z(R_3^1(p+m-k-1, l+q-3, S_{k+1}^k)) \\ &\geq Z(R_3^1(n-k-4, 3, S_{k+1}^k)). \end{aligned}$$

Case 2 $l = 2$ and $q > 3$.

The result is the same as in Case 1.

Case 3 $l = 2$ and $q = 3$.

Then by Lemma 3.8, $Z(R_2^1(p, 3, S_m^k)) \geq Z(R_2^1(n-k-3, 3, S_{k+1}^k))$.

Combining the above arguments, we have $Z(G) \geq \min\{Z(R_3^1(n-k-4, 3, S_{k+1}^k)), Z(R_2^1(n-k-3, 3, S_{k+1}^k))\}$ for any $G \in G(0, k)$ when $2 \leq k \leq n-6$.

Suppose $k = n-6$. Then by $p, q \geq 3$, $l \geq 2$ and $n = p+q+l+k-2$, we have $l = 2$, $p = q = 3$. Thus $Z(G) \geq Z(R_2^1(3, 3, S_{n-5}^{n-6})) = 20n-28$.

Suppose $2 \leq k \leq n-7$. By Lemma 3.6, we have $Z(R_3^1(n-k-4, 3, S_{k+1}^k)) - Z(R_2^1(n-k-3, 3, S_{k+1}^k)) = (2k-3)(F_{n-k-4} - 2F_{n-k-5}) - F_{n-k-4} < 0$. Thus $Z(G) \geq Z(R_3^1(n-k-4, 3, S_{k+1}^k)) = 6kF_{n-k-4} + 10F_{n-k-3} + 2F_{n-k-5}$.

Let m be positive integers, P_m be a path on m vertices, $v \in V(P_m)$ and $d(v) = 1$. Take $R_l^i(p, q, P_m) = (S_l(p, q), u_i) \triangle (P_m, v)$ $(i = 1, 2, 3, 4, 5)$, then $R_l^i(p, q, P_m) \in G^0(p, q, 1)$.

Similarly to the proof of Lemmas 3.5 and 3.6, by (1) of Proposition 2.6, we have

Lemma 3.11 *Suppose $G \in G^0(p, q, 1)$ on n vertices, and P_l is the path connecting C_p and C_q with length $l-1$. Then $Z(G) \geq Z(R_l^1(p, q, P_m))$ or $Z(G) \geq Z(R_l^4(p, q, P_m))$.*

Lemma 3.12 *Let l, m, p, q be positive integers with $l \geq 2$, $p, q \geq 3$, $R_l^1(p, q, P_m)$ and $u_i (1 \leq i \leq 5)$ be defined as above. Then*

$$Z(R_l^1(p, q, P_m)) = F_pF_mf(l, q) + [F_pF_{m-1} + 2F_{p-1}F_m]f(l-1, q).$$

Remark 3.13 For $k = 1$, similarly to the proof of Lemmas 3.7–3.9 and Theorem 3.10, we can show that $R_3^1(n-5, 3, P_2)$ is the graph with the smallest Hosoya index in $G(0, 1)$.

By Theorem 3.10 and Remark 3.13, we have

Lemma 3.14 *Let n, k be positive integers. Then*

(1) $Z(R_3^1(n-5, 3, P_2)) > Z(R_3^1(n-6, 3, S_3^2))$.

(2) $Z(R_3^1(n-k-4, 3, S_{k+1}^k)) > Z(R_3^1(n-k-5, 3, S_{k+2}^{k+1}))$ *for* $2 \le k \le n-8$.

(3) $Z(R_3^1(3, 3, S_{n-6}^{n-7})) > Z(R_2^1(3, 3, S_{n-5}^{n-6}))$.

Theorem 3.15 *Let G be a bicyclic graph on n vertices with the two cycles having no common vertices. Then $Z(G) \ge 8n - 28$, with the equality holding if and only if $G \cong R_2^1(3, 3, S_{n-5}^{n-6})$.*

4. The graph with the smallest Hosoya index in $G(1, k)$

In this section, we will characterize the graph on n vertices with the smallest Hosoya index in $G(1, k)$.

Let $p(\ge 3), q(\ge 3)$ be positive integers, $S(p, q)$ be the graph on $p + q - 1$ vertices, obtained by connecting C_p and C_q with a common vertex v_1 (see Figure 7). That is, $S(p, q) = (C_p, x) \triangle (C_q, y)$, where $x \in V(C_p)$ and $y \in V(C_q)$, denote x and y by v_1. For convenience, we let $v_2 \in V(S(p, q)) \backslash V(C_q)$, $v_3 \in V(S(p, q)) \backslash V(C_p)$, $v_1^* \ne v_2$ and $v_1^* (\in V(C_p) \backslash V(P_{v_1 v_2}))$ be adjacent to v_1, where $P_{v_1 v_2}$ is the shortest path from v_1 to v_2 of C_p.

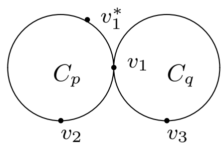


Figure 7 Graph $S(p, q)$

Lemma 4.1 *For $1 \le i \le 3$, we have* $Z(S(p, q) - v_i) < \frac{3}{2} \sum_{x \in N_{S(p,q)}(v_i)} Z(S(p, q) - \{x, v_i\})$.

Proof There are three cases.

Case 1 $i = 1$.

By Lemma 2.1 and $F_p \le 2F_{p-1}$ for $p \ge 3$,

$$\begin{aligned} & Z(S(p,q) - v_1) - \frac{3}{2} \sum_{x \in N_{S(p,q)}(v_1)} Z(S(p,q) - \{x, v_1\}) \\ & < Z(S(p,q) - v_1) - \sum_{x \in N_{S(p,q)}(v_1)} Z(S(p,q) - \{x, v_1\}) \\ & = Z(P_{p-1})Z(P_{q-1}) - [2Z(P_{p-2})Z(P_{q-1}) + 2Z(P_{p-1})Z(P_{q-2})] \\ & = (F_p - 2F_{p-1})F_q - 2F_pF_{q-1} < 0. \end{aligned}$$

Case 2 $i = 2$.

Let $d(v_1, v_2) = s - 1$. Then $s \ge 2$.

Subcase 2.1 $s = 2$.

$$\begin{aligned}
&2Z(S(p,q)-v_2) - 3\sum_{x\in N_{S(p,q)}(v_2)} Z(S(p,q)-\{x,v_2\})\\
&= 2Z(P(p-1,1,C_q,v_1)) - 3Z(P(p-2,1,C_q,v_1)) - 3Z(P_{q-1})Z(P_{p-2})\\
&= 2f(p-1,q) - 3f(p-2,q) - 3F_qF_{p-1}\\
&= [f(p-3,q) - f(p-2,q)] + [2F_{q-1}F_{p-3} + F_qF_{p-2} - 3F_qF_{p-1}] < 0.
\end{aligned}$$

Subcase 2.2 $s \geq 3$.

Let $e = v_1v_1^*$. By Lemma 2.1 and Propsition 2.6,

$$\begin{aligned}
&Z(S(p,q)-v_2) - \frac{3}{2}\sum_{x\in N_{S(p,q)}(v_2)} Z(S(p,q)-\{x,v_2\})\\
&< Z(S(p,q)-v_2) - \sum_{x\in N_{S(p,q)}(v_2)} Z(S(p,q)-\{x,v_2\})\\
&= [Z(S(p,q)-v_2-e) + Z(S(p,q)-\{v_2,v_1,v_1^*\})] -\\
&\quad [\sum_{x\in N_{S(p,q)}(v_2)} Z(S(p,q)-\{x,v_2\}-e) + \sum_{x\in N_{S(p,q)}(v_2)} Z(S(p,q)-\{x,v_2,v_1,v_1^*\})]\\
&= Z(P(s-1,1,C_q,v_1))Z(P_{p-s}) + Z(P_{s-2})Z(P_{p-s-1})Z(P_{q-1}) -\\
&\quad [Z(P(s-2,1,C_q,v_1))Z(P_{p-s}) + Z(P_{q-1})Z(P_{s-3})Z(P_{p-s-1})] -\\
&\quad [Z(P(s-1,1,C_q,v_1))Z(P_{p-s-1}) + Z(P_{q-1})Z(P_{s-2})Z(P_{p-s-2})]\\
&= [F_{p-s-1}f(s-3,q) - F_{p-s}f(s-2,q)] + [F_{p-s-2}F_{s-3} - F_{p-s-1}F_{s-2}]F_q < 0.
\end{aligned}$$

Case 3 $i = 3$. It is similar to Case 2.

Combining the above arguments, we prove the result.

By Lemmas 2.9 and 4.1, the following corollary holds:

Corollary 4.2 *Let $s(\geq 3), t, k, p(\geq 3), q(\geq 3)$ be positive integers with $1 \leq t \leq s-1$, $P(n,1,H,v,t,k)$, $S(p,q)$ be defined as before. Then for $1 \leq i \leq 3$,*

$$Z(P(s,1,S(p,q),v_i,1,k)) \leq Z(P(s,1,S(p,q),v_i,t,k))$$

with the equality holding if and only if $t = 1$.

Let $n, m, k, p(\geq 3), q(\geq 3)$ be positive integers with $2 \leq k \leq m-1$ and $n = p+q+m-2$, $v \in V(T_m^k)$ and $d(v) \geq 2$. Take $S_i(p,q,T_m^k) = (S(p,q),v_i) \triangle (T_m^k, v)$ $(i = 1,2,3)$ (see Figure 8), then $S_i(p,q,T_m^k) \in G^1(p,q,k)$.

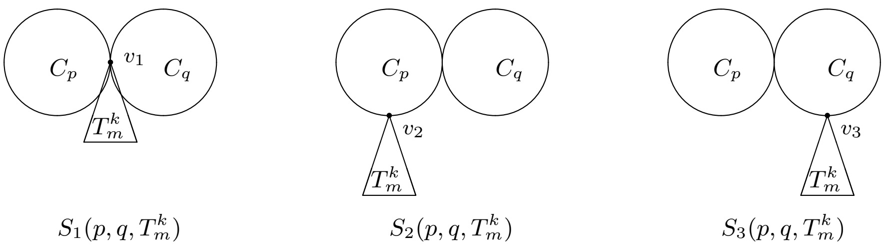


Figure 8 $S_i(p,q,T_m^k)(i = 1,2,3)$

Lemma 4.3 *Let m, k, p, q, t be positive integers with $p, q \geq 3$, $2 \leq k \leq m-1$, $S(p,q)$, v_i, $S_i(p,q,T_m^k)$, $P(m-k+1, 1, S(p,q), v_i, t, k-1)$ be defined as before for $1 \leq i \leq 3$. Then for any i $(1 \leq i \leq 3)$, there exists some integer t with $1 \leq t \leq m-k$ such that*

$$Z(S_i(p,q,T_m^k)) \geq Z(P(m-k+1, 1, S(p,q), v_i, t, k-1)).$$

Proof For any i $(1 \leq i \leq 3)$, repeating Transformations A and B on $S_i(p,q,T_m^k)$, we can get a graph $P(m-k+1, 1, S(p,q), v_i, t, k-1)$. By Lemmas 2.2 and 2.3, $Z(S_i(p,q,T_m^k)) \geq Z(P(m-k+1, 1, S(p,q), v_i, t, k-1))$.

Note that $S_i(p,q,S_m^k) = P(m-k+1, 1, S(p,q), v_i, 1, k-1)$, by Corollary 4.2 and Lemma 4.3, we can get the following corollary immediately.

Corollary 4.4 *Let $1 \leq i \leq 3$. We have $Z(S_i(p,q,T_m^k)) \geq Z(S_i(p,q,S_m^k))$, with the equality holding if and only if $T_m^k = S_m^k$.*

Lemma 4.5 *Suppose $G \in G^1(p,q,k)$ on n vertices. Then $Z(G) \geq Z(S_1(p,q,S_m^k))$.*

Proof It is obvious that there exist some i $(1 \leq i \leq 3)$ and some tree T_m^k such that $Z(G) \geq Z(S_i(p,q,T_m^k))$ by Transformation A on G. Then we only need to show $Z(S_i(p,q,S_m^k)) > Z(S_1(p,q,S_m^k))$ for $i = 2, 3$ by Corollary 4.4.

Note that $S_i(p,q,S_m^k) = P(m-k+1, 1, S(p,q), v_i, 1, k-1)$, we only need to show the following inequalities by Lemma 2.10:

$$Z(S(p,q) - v_1) < Z(S_l(p,q) - v_2), \tag{4.1}$$

$$Z(S_l(p,q) - v_1) < Z(S_l(p,q) - v_3). \tag{4.2}$$

Since the proof of (4.2) is similar to that of (4.1) by the symmetry of C_p and C_q, we only show (4.1). Let $d(v_1, v_2) = s-1$. Then $s \geq 2$.

Case 1 $s = 2$.

$$\begin{aligned} Z(S(p,q) - v_1) - Z(S(p,q) - v_2) &= Z(P_{p-1})Z(P_{q-1}) - Z(P(p-1, 1, C_q, v_1)) \\ &= -2F_{p-1}F_{q-1} < 0. \end{aligned}$$

Case 2 $s \geq 3$.

Let $e = v_1 v_1^*$. By Lemma 2.1 and $F_n = F_k F_{n-k+1} + F_{k-1} F_{n-k}$ for $1 \leq k \leq n$, we have

$$\begin{aligned} &Z(S(p,q) - v_1) - Z(S(p,q) - v_2) \\ &\quad = Z(S(p,q) - v_1) - [Z(S(p,q) - v_2 - e) + Z(S(p,q) - \{v_2, v_1, v_1^*\})] \\ &\quad = Z(P_{p-1})Z(P_{q-1}) - Z(P_{p-s})Z(P(s-1, 1, C_q, v_1)) - Z(P_{p-s-1})Z(P_{s-2})Z(P_{q-1}) \\ &\quad = -2F_{p-s+1}F_{s-1}F_{q-1} < 0. \end{aligned}$$

The proof of the following Lemma 4.6 is similar to the proof of Lemma 3.6.

Lemma 4.6 *Let m, k, p, q be positive integers with $p, q \geq 3$ and $2 \leq k \leq m-1$, $S_1(p,q,T_m^k)$*

and $v_i(1 \le i \le 3)$ *be defined as above. Then*

$$Z(S_1(p,q,S_m^k)) = kF_pF_qF_{m-k+1} + 2F_{p-1}F_qF_{m-k+1} + 2F_pF_{q-1}F_{m-k+1} + F_pF_qF_{m-k}.$$

Lemma 4.7 *Let* m,k,p,q *be positive integers with* $p,q \ge 3$, $p+q-4 \ge 3$ *and* $2 \le k \le m-1$. *Then* $Z(S_1(p,q,S_m^k)) \ge Z(S_1(4,p+q-4,S_m^k))$, *with the equality holding if and only if* $S_1(p,q,S_m^k) \cong S_1(4,p+q-4,S_m^k)$.

Proof We will complete the proof by the following two cases.

Case 1 $p \ge 4$.

By $F_n = F_kF_{n-k+1} + F_{k-1}F_{n-k}$ for $1 \le k \le n$,

$$F_pF_q - F_4F_{p+q-4} = [F_{p-1}+F_{p-2}][2F_{q-2}+F_{q-3}] - 3[F_{p-1}F_{q-2}+F_{p-2}F_{q-3}] = F_{p-4}[F_{q-2}-F_{q-3}];$$

$$F_{p-1}F_q - F_3F_{p+q-4} = F_{p-1}[2F_{q-2}+F_{q-3}] - 2[F_{p-1}F_{q-2}+F_{p-2}F_{q-3}] = -F_{p-4}F_{q-3}.$$

Thus by Lemma 4.6,

$$\begin{aligned} &Z(S_1(p,q,S_m^k)) - Z(S_1(4,p+q-4,S_m^k)) \\ &= [k(F_pF_q - F_4F_{p+q-4}) + 2(F_{p-1}F_q - F_3F_{p+q-4}) + 2(F_pF_{q-1} - F_4F_{p+q-5})]F_{m-k+1} + \\ &\quad [F_pF_q - F_4F_{p+q-4}]F_{m-k} \\ &= F_{p-4}[F_{q-2} - F_{q-3}][(k-2)F_{m-k+1} + F_{m-k}] \ge 0. \end{aligned}$$

The equality holds if and only if $p = 4$ or $q = 4$.

Case 2 $p = 3$.

Then $q \ge 4$ by $p+q-4 \ge 3$. By Lemma 4.6,

$$\begin{aligned} &Z(S_1(p,q,S_m^k)) - Z(S_1(4,p+q-4,S_m^k)) \\ &= [k(F_3F_q - F_4F_{q-1}) + 2(F_2F_q - F_3F_{q-1}) + 2(F_3F_{q-1} - F_4F_{q-2})]F_{m-k+1} + \\ &\quad [F_3F_q - F_4F_{q-1}]F_{m-k} \\ &= F_{q-4}[(k-2)F_{m-k+1} + F_{m-k}] \ge 0. \end{aligned}$$

The equality holds if and only if $q = 4$.

Combining the two cases, we obtain the equality holds if and only if $S_1(p,q,S_m^k) \cong S_1(4,p+q-4,S_m^k)$.

Lemma 4.8 *Let* m,k,p,q *be positive integers with* $p,q \ge 3$ *and* $2 \le k \le m-1$. *Then* $Z(S_1(p,q,S_m^k)) \ge Z(S_1(p,q+m-k-1,S_{k+1}^k))$, *with the equality holding if and only if* $m = k+1$.

Proof By $F_n = F_kF_{n-k+1} + F_{k-1}F_{n-k}$ for $1 \le k \le n$,

$$F_{q+m-k-1} = F_{q-1}F_{m-k+1} + F_{q-2}F_{m-k}; \quad F_{q+m-k-2} = F_{q-2}F_{m-k+1} + F_{q-3}F_{m-k}.$$

$$F_qF_{m-k+1} - F_{q+m-k-1} = F_qF_{m-k+1} - [F_{q-1}F_{m-k+1} + F_{q-2}F_{m-k}] = F_{q-2}F_{m-k-1}.$$

Then by Lemma 4.6,

$$Z(S_1(p,q,S_m^k)) - Z(S_1(p,q+m-k-1,S_{k+1}^k))$$

$$= (kF_p + 2F_{p-1})[F_qF_{m-k+1} - F_{q+m-k-1}] + 2F_p[F_{q-1}F_{m-k+1} - F_{q+m-k-2}] + F_p[F_qF_{m-k} - F_{q+m-k-1}]$$
$$= [(kF_{q-2} + 2F_{q-3} - F_{q-1})F_p + 2F_{p-1}F_{q-2}]F_{m-k-1} \geq 0.$$

The equality holds if and only if $m = k + 1$.

By Lemmas 4.1–4.6, we have the following theorem.

Theorem 4.9 *Let n, k be positive integers with $2 \leq k \leq n-6$, $G \in \mathcal{G}(n, n+1, k)$ be a bicyclic graph on n vertices and k pendent vertices with the two cycles having exactly one common vertices. Then we have*

(1) If $2 \leq k \leq n-6$, then $Z(G) \geq (3k+7)F_{n-k-3} + 6F_{n-k-4}$, with the equality holding if and only if $G \cong S_1(4, n-k-3, S_{k+1}^k)$.

(2) If $k = n-5$, then $Z(G) \geq 4n-8$, with the equality holding if and only if $G \cong S_1(3, 3, S_{n-4}^{n-5})$.

Proof Let p, q be positive integers with $p, q \geq 3$ and $G \in G^1(p, q, k)$ on n vertices. Suppose the two cycles in G are connected by a common vertex v_1. Then there exist $i \in \{1, 2, 3\}$ and some tree T_m^k where $2 \leq k \leq m-1$ and $m = n-p-q+2$ such that $Z(G) \geq Z(S_i(p, q, T_m^k))$ by Transformation A.

Thus by Corollary 4.4 and Lemma 4.5,

$$Z(G) \geq Z(S_i(p, q, T_m^k) \geq Z(S_i(p, q, S_m^k) \geq Z(S_1(p, q, S_m^k).$$

Case 1 $p + q \geq 7$. Then by Lemmas 4.6–4.8,

$$Z(S_1(p, q, S_m^k)) \geq Z(S_1(4, p+q-4, S_m^k)) \geq Z(S_1(4, n-k-3, S_{k+1}^k)) = (3k+7)F_{n-k-3} + 6F_{n-k-4}.$$

Case 2 $p = q = 3$.

By Lemmas 4.6 and 4.8, $Z(S_1(3, 3, S_m^k)) \geq Z(S_1(3, n-k-2, S_{k+1}^k))$.

Combining the above arguments and Lemma 4.7, we have $Z(G) \geq Z(S_1(4, n-k-3, S_{k+1}^k))$ when $2 \leq k \leq n-6$ and $Z(G) \geq Z(S_1(3, 3, S_{n-4}^{n-5})) = 4n-8$ when $k = n-5$.

Let m be a positive integer, P_m be a path on m vertices, $v \in V(P_m)$ and $d(v) = 1$. Take $S_i(p, q, P_m) = (S(p, q), v_i) \bigtriangleup (P_m, v)$ $(i = 1, 2, 3)$, then $S_i(p, q, P_m) \in G^1(p, q, 1)$.

It is obvious that Lemmas 4.5−4.6 and Lemma 4.8 hold for $S_1(p, q, P_m)$, and

$$Z(S_1(p, q, P_2)) = 2F_pF_q + 2F_{p-1}F_q + 2F_pF_{q-1}.$$

Similarly to the proof of Lemma 4.7, we can show $Z(S_1(p, q, P_2)) = Z(S_1(3, p+q-3, P_2))$. Then we have the following remark.

Remark 4.10 For $k = 1$, $S_1(p, n-p, P_2)$ is the graph on n vertices with the smallest Hosoya index in $G(1, 1)$ when $p, q \geq 3$ and $Z(S_1(p, n-p, P_2)) = Z(S_1(4, n-4, P_2)) = 4F_{n-4} + 6F_{n-3}$.

By Theorem 4.9 and Remark 4.10, we have

Lemma 4.11 *Let n, k be positive integers. Then*

(1) $Z(S_1(4,n-4,P_2)) > Z(S_1(4,n-5,S_3^2))$.

(2) $Z(S_1(4,n-k-3,S_{k+1}^k)) > Z(S_1(4,n-k-4,S_{k+2}^{k+1}))$ *for* $2 \le k \le n-7$.

(3) $Z(S_1(4,3,S_{n-5}^{n-6})) > Z(S_1(3,3,S_{n-4}^{n-5}))$.

Theorem 4.12 *Let G be a bicyclic graph on n vertices with the two cycles having common vertices. Then $Z(G) \ge 4n-8$, with the equality holding if and only if $G \cong S_1(3,3,S_{n-4}^{n-5})$.*

5. The graph with the smallest Hosoya index in $G(l,k)$

In this section, we will characterize the graph on n vertices with the smallest Hosoya index in $G(l,k)$ for $l \ge 2$. Since the proofs of the following results are similar to those of the above results in Section 3 or 4, so we ignore them.

Let $p(\ge 3), q(\ge 3)$ be positive integers, and $S(p,q,l)$ a graph on $p+q-l$ vertices, with the two cycles C_p and C_q having l common vertices (see Figure 9). For convenience, we let $w_1 = z_1$, $w_2 \in \{x_1, x_2, \ldots, x_{p-l}\}$, $w_3 \in \{y_1, y_2, \ldots, y_{q-l}\}$, and $w_4 \in \{z_2, \ldots, z_{l-1}\}$ if $l \ge 3$.

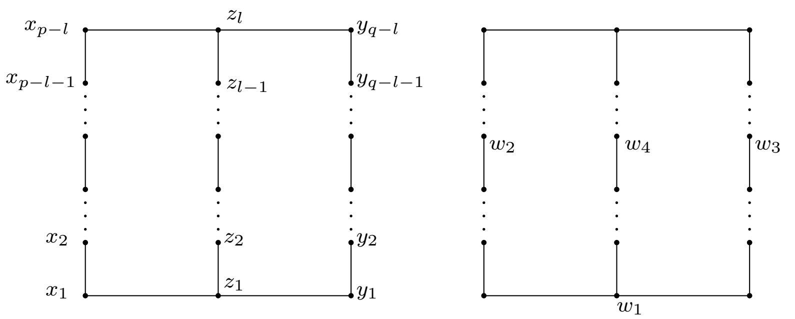


Figure 9 $S(p,q,l)$

Lemma 5.1 *For $1 \le i \le 4$, we have $Z(S(p,q,l)-w_i) < \frac{3}{2}\sum_{x \in N_{S(p,q,l)}(w_i)} Z(S(p,q,l)-\{x,w_i\})$.*

By Lemmas 2.9 and 5.1, the following corollary holds:

Corollary 5.2 *Let $n(\ge 3), t, k$ be positive integers with $1 \le t \le n-1$, $P(n,1,H,v,t,k)$, $S(p,q,l)$ be defined as before. Then for any i $(1 \le i \le 4)$,*

$$Z(P(n,1,S(p,q,l),w_i,1,k)) \le Z(P(n,1,S(p,q,l),w_i,t,k))$$

with the equality holding if and only if $t = 1$.

Let m, k be positive integers with $2 \le k \le m-1$, $v \in V(T_m^k)$ and $d(v) \ge 2$. Take $\theta^i(p,q,l,T_m^k) = (S(p,q,l),w_i) \triangle (T_m^k, v)$ $(i = 1,2,3,4)$ (see Figure 10), then $\theta^i(p,q,l,T_m^k) \in G^l(p,q,k)$.

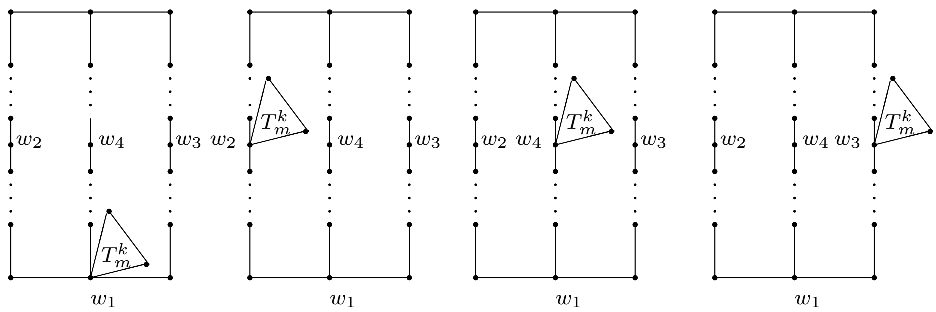


Figure 10 $\theta^i(p,q,l,T_m^k)$ $(i=1,2,3,4)$

Lemma 5.3 *Let m,k,p,q,t be positive integers with $p,q\geq 3$ and $2\leq k\leq m-1$, $S(p,q,l)$, w_i, $\theta^i(p,q,l,T_m^k)$, $P(m-k+1,1,S(p,q,l),w_i,t,k-1)$ be defined as before for $1\leq i\leq 4$. Then for any i $(1\leq i\leq 4)$, there exists some integer t with $1\leq t\leq m-k$ such that*

$$Z(\theta^i(p,q,l,T_m^k))\geq Z(P(m-k+1,1,S(p,q,l),w_i,t,k-1)).$$

Note that $\theta^i(p,q,l,S_m^k)=P(m-k+1,1,S(p,q,l),w_i,1,k-1)$, by Corollary 5.2 and Lemma 5.3, we can get the following corollary immediately.

Corollary 5.4 *Let $1\leq i\leq 4$. We have $Z(\theta^i(p,q,l,T_m^k)\geq Z(\theta^i(p,q,l,S_m^k)$, with the equality holding if and only if $T_m^k=S_m^k$.*

Lemma 5.5 *Suppose $G\in G^l(p,q,k)$ on n vertices, and P_l is the common path of C_p and C_q. Then $Z(G)\geq Z(\theta^1(p,q,l,S_m^k))$.*

Lemma 5.6 *Let m,k,p,q,l be positive integers with $2\leq k\leq m-1$, $p,q\geq 3$ and $l\geq 2$, $\theta^1(p,q,l,S_m^k)$ and w_1 be defined as above. Take $F_{-1}=1$, then*

$$Z(\theta^1(p,q,l,S_m^k))=rkF_{m-k+1}+rF_{m-k}+sF_{m-k+1},$$

where

$$r=F_{p+q-2l+2}F_{l-1}+F_{p-l+1}F_{l-2}F_{q-l+1},$$

$$s=2F_{p+q-2l+1}F_{l-1}+[F_{p-l}F_{q-l+1}+F_{p-l+1}F_{q-l}+F_{p+q-2l+2}]F_{l-2}+F_{p-l+1}F_{q-l+1}F_{l-3}.$$

Lemma 5.7 *Let m,k,p,q,l be positive integers with $2\leq k\leq m-1$, $p,q\geq 3$ and $l\geq 2$. Then $Z(\theta^1(p,q,l,S_m^k))\geq Z(\theta^1(l+1,q+p-l-1,l,S_m^k))$, with equality holding if and only if $\theta^1(p,q,l,S_m^k))\cong\theta^1(l+1,q+p-l-1,l,S_m^k)$.*

For the symmetry of P_{p-l}, P_{q-l} and P_l, the following lemma holds:

Lemma 5.8 *Let m,k,p,q,l be positive integers with $2\leq k\leq m-1, 2\leq l$. Then*

$$Z(\theta^1(l+1,q,l,S_m^k))\geq Z(\theta^1(q,q,q-1,S_m^k)).$$

Lemma 5.9 *Let m,k,p,q,l be positive integers with $2\leq k\leq m-1$, $p,q\geq 3$ and $l\geq 2$. Then $Z(\theta^1(l+1,l+1,l,S_m^k))\geq Z(\theta^1(l+m-k+2,l+m-k+2,l+m-k+1,S_{k+1}^k))$.*

Theorem 5.10 *Let n, k be positive integers with $2 \leq k \leq n-4$, $G \in \mathcal{G}(n, n+1, k)$ be a bicyclic graph on n vertices and k pendent vertices with the two cycles having exactly at least two common vertices. Then $Z(G) \geq 2F_{n-k}+(k+1)F_{n-k-1}+kF_{n-k-3}$, with the equality holding if and only if $G \cong \theta^1(n-k-1, n-k-1, n-k-2, S^k_{k+1})$.*

Remark 5.11 For $k = 1$, similarly to the proofs of Lemmas 5.7–5.9 and Theorem 5.10, we can show that $\theta^1(n-2, n-2, n-3, P_2)$ is the graph with the the smallest Hosoya index in $G(l, 1)$ and $Z(\theta^1(n-2, n-2, n-3, P_2)) = 2F_n + F_{n-4}$.

By Theorem 5.10 and Remark 5.11, we have

Lemma 5.12 *Let n, k be positive integers. Then*

(1) $Z(\theta^1(n-2, n-2, n-3, P_2)) > Z(\theta^1(n-3, n-3, n-4, S^2_3))$.

(2) $Z(\theta^1(n-k-1, n-k-1, n-k-2, S^k_{k+1})) > Z(\theta^1(n-k-2, n-k-2, n-k-3, S^{k+1}_{k+2}))$ for $2 \leq k \leq n-4$.

Theorem 5.13 *Let G be a bicyclic graph on n vertices with the two cycles having at least two common vertices. Then $Z(G) \geq 3n-4$, with the equality holding if and only if $G \cong \theta^1(3, 3, 2, S^{n-4}_{n-3})$.*

6. The graph with the smallest Hosoya index in $\mathcal{G}(n, n+1, k)$ and $\mathcal{G}(n, n+1)$

Let $\mathcal{G}(n, n+1)$ be the set of bicyclic graphs on n vertices. By Theorems 3.10, 3.15, 4.9, 4.12, 5.10 and 5.13, we obtain the extremal graphs with the smallest Hosoya index in $\mathcal{G}(n, n+1, k)$ and $\mathcal{G}(n, n+1)$.

Theorem 6.1 *Let G be a connected graph on n vertices in $\mathcal{G}(n, n+1, k)$. Then*

(1) For $k = 1$, $Z(G) \geq 4F_{n-2} + 2F_{n-3}$, with the equality holding if and only if $G \cong S_1(4, n-4, P_2)$.

(2) For $2 \leq k \leq n-6$, $Z(G) \geq (3k+7)F_{n-3-k} + 6F_{n-4-k}$, with the equality holding if and only if $G \cong S_1(4, n-k-3, S^k_{k+1})$.

(3) For $k = n-5$, $Z(G) \geq 4n-8$, with the equality holding if and only if $G \cong S_1(3, 3, S^{n-5}_{n-4})$.

(4) For $k = n-4$, $Z(G) \geq 3n-4$, with the equality holding if and only if $G \cong \theta^1(3, 3, 2, S^{n-4}_{n-3})$.

Theorem 6.2 ([13]) *Let G be a connected graph in $\mathcal{G}(n, n+1)$. Then $Z(G) \geq 3n-4$, with the equality holding if and only if $G \cong \theta^1(3, 3, 2, S^{n-4}_{n-3})$.*

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