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Extremal Bicyclic Graphs with Respect to Permanental Sums and Hosoya Indices

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Abstract: Graph polynomials is one of the important research directions in mathematical chemistry. The coefficients of some graph polynomials, such as matching polynomial and permanental polynomial, are related to structural properties of graphs. The Hosoya index of a graph is the sum of the absolute value of all coefficients for the matching polynomial. And the permanental sum of a graph is the sum of the absolute value of all coefficients of the permanental polynomial. In this paper, we characterize the second to sixth minimal Hosoya indices of all bicyclic graphs. Furthermore, using the results, the second to sixth minimal permanental sums of all bicyclic graphs are also characterized.

Keywords: permanental polynomial; matching polynomial; permanental sum; Hosoya index

MSC: 05C92; 92E10

1. Introduction

Let $G = (V(G), E(G))$ be a graph. The vertex set and edge set of G are denoted by $V(G) = \{v_1, v_2, ..., v_n\}$ and $E(G) = \{e_1, e_2, ..., e_m\}$, respectively. Denote by $A(G) = (a_{ij})_{n\times n}$ the adjacency matrix of graph G which is a symmetric matrix such that $a_{ij} = 1$ if vertices v_i and v_j are adjacent and 0 otherwise.

The *permanent* of matrix $M = (a_{ij})_{n\times n}$ is defined as

$$\mathrm{per}(M) = \sum_{\Delta} \prod_{i=1}^{n} a_{i\Delta(i)},$$

here the sum is taken over all permutations Δ of $\{1, 2, 3, 4, \ldots, n-1, n\}$. Computational complexity is a branch of theoretical computer science. #P is the class of functions that can be computed by counting TMs of polynomial time complexity. Valiant [1] proved that calculating $\mathrm{per}(M)$ is #P-complete. For a more detailed explanation of #P-complete, we refer readers to [2].

The *permanental polynomial* of G, denoted by $\pi(G, x)$, is defined as

$$\pi(G, x) = \mathrm{per}(xI - A(G)) = \sum_{k=0}^{n} b_k(G)x^{n-k},$$

here I denotes the $n \times n$ identity matrix. The permanental polynomial has been considered widely in chemical literature [3–5]; interested readers can consult the sources for themselves.

Graph G is called a *basic graph* if each of its components is a cycle or an isolated edge. For an integer $r \geq 1$, assume that $S_r(G)$ denotes the set of all basic subgraphs H of G on r

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Citation: Wu, T.; Bai, Y.; Xu, S. Extremal Bicyclic Graphs with Respect to Permanental Sums and Hosoya Indices. *Axioms* **2024**, *13*, 330. https://doi.org/10.3390/axioms13050330

Academic Editor: Fabio Caldarola

Received: 2 March 2024
Revised: 14 May 2024
Accepted: 14 May 2024
Published: 16 May 2024

vertices, and suppose that $c(H)$ is the number of cycles in a graph H. Merris et al. [6] gave the computing formula on the coefficients of $\pi(G,x)$ as follows,

$$b_r(G) = (-1)^r \sum_{H \in S_r(G)} 2^{c(H)}, \ 1 \le r \le n.$$

with $b_0(G) = 1$.

The sum of $|b_r(G)|$ is called the *permanental sum* of G, written as $PS(G)$, and is expressed as follows:

$$PS(G) = \sum_{r=0}^{n} |b_r(G)| = 1 + \sum_{r=1}^{n} \sum_{H \in S_r(G)} 2^{c(H)}.$$

Wu and So [7] introduced the matrix form expression for $PS(G)$:

$$PS(G) = \mathrm{per}(I + A(G)).$$

Combining Valiant's results, we know that calculating $PS(G)$ is #P-complete.

Tong [8] first investigated the permanental sum of a graph. Xie et al. [9] captured a fullerene $C_{50}(D_{5h})$. Tong calculated the permanental sums of all 271 fullerenes in C_{50}. He pointed out that $PS(C_{50}(D_{5h}))$ attains the minimum among all 271 fullerenes. And he also indicated that the permanental sum would be closely related to the stability of molecular graphs. Recently, the permanental sums of graphs have received a lot of attention from researchers. Wu and Lai [10] presented the basic properties of the permanental sums of graphs. Li et al. [11] characterized the extremal hexagonal chains with respect to permanental sums. Li and Wei [12] characterized the extremal octagonal chains with respect to permanental sums. More results on permanental sums are available in the literature [7,13,14].

r-matchings of G are r isolated edges with no shared endpoints in G. The number of r-matchings in G is denoted by $m(G,r)$. The *matching polynomial* of G, written as $\mu(G,x)$, is expressed by

$$\mu(G,x) = \sum_{r \ge 0} (-1)^r m(G,r) x^{n-2r}.$$

Matching polynomials have been extensively studied; specifically, see the literature studies [15,16].

The sum of $|m(G,r)|$ is called the *Hosoya index* of graph G, denoted by $Z(G)$. And it is expressed as follows,

$$Z(G) = \sum_{r \ge 0} m(G,r).$$

An application of $Z(G)$ was introduced in 1971 by the chemist Hosoya. And he used the Hosoya index to describe the thermodynamic properties of saturated hydrocarbons. For some related work on the Hosoya index, see [17,18].

Recently, the first author found an important relation between the permanental sum and the Hosoya index as follows.

Theorem 1 ([19])**.** *Assume that G is a graph. And suppose that $\mathscr{C}$ is the set whose elements G' are disjoint unions of cycles in G. Then*

$$PS(G) = Z(G) + \sum_{G' \in \mathscr{C}} 2^{c(G')} Z(G - G'),$$

here $G - G'$ is a graph obtained by deleting all vertices and edges of G' in G.

An important direction is to characterize the graphs with an extremal Hosoya index and permanental sum in a given type of graph. A *bicyclic graph* G is a connected simple graph of order n and size $n+1$. Deng [20] determined the bicyclic graph with the smallest Hosoya index. Wu and Das [21] characterized the bicyclic graphs with the smallest permanental sum. In this article, our aim is to determine which bicyclic graphs have the second, the third, the fourth, the fifth and the sixth minimal Hosoya indices and permanental sums.

This article is organized as follows. In Section 2, we introduce some preliminaries and some lemmas on permanental sums and Hosoya indices. We characterize the second to the sixth bicyclic graphs with the smallest Hosoya index in Section 3. In Section 4, using the results in Section 3, we also determine the second to the sixth bicyclic graphs with the smallest permanental sums. Finally, We summarize the main results of this article.

2. Some Preliminaries

Suppose that $\mathscr{B}_n$ is the collection of all bicyclic graphs of order n vertices. By the construction of bicyclic graphs, we know that $\mathscr{B}_n$ consists of three classes of graphs: the first class, written as $\mathscr{B}_n^1$, is the set of those graphs, each of which contains $B_1(p,q)$ as the vertex-induced subgraph for some p and q, see Figure 1; the second class, written as $\mathscr{B}_n^2$, is the collection of those, graphs each of which contains $B_2(p,q,r)$ as the vertex-induced subgraph for some p, q and r, see Figure 1; the third class, written as $\mathscr{B}_n^3$, is the collection of those graphs, each of which contains $B_3(p,q,r)$ as the vertex-induced subgraph for some p, q and r, see Figure 1. Then, we know that $\mathscr{B}_n = \mathscr{B}_n^1 \cup \mathscr{B}_n^2 \cup \mathscr{B}_n^3$.

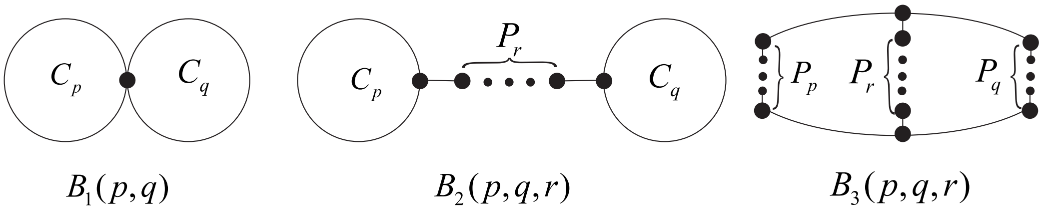

Figure 1. Bicyclic graphs $B_1(p,q)$, $B_2(p,q,r)$ and $B_3(p,q,r)$.

Now, we present some graph transformations that do not increase the Hosoya indices of graphs.

Definition 1. *Suppose that* $uv \in E(G)$ *and* $N_G(u) = \{v, w_1, w_2, \ldots, w_s\}$, *where* $d(w_i) = 1 (1 \le i \le s)$. *Let* $G^* = G - \{uw_1, uw_2, \ldots, uw_s\} + \{vw_1, vw_2, \ldots, vw_s\}$, *see Figure 2. We say the transformation from* G *to* G^* *in Figure 2 is of type* **I**.

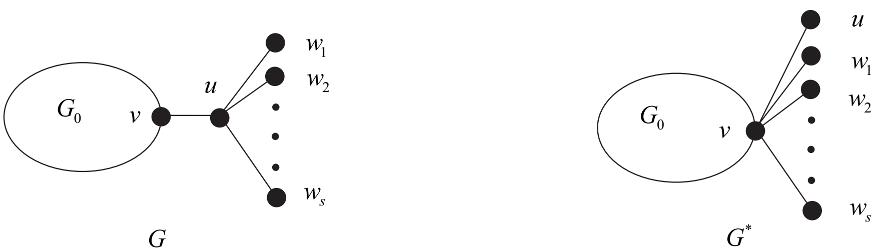

Figure 2. Graphs G and G^*.

Lemma 1 ([20]). *Assume that* G *and* G^* *are two graphs of order* n *defined in Definition 1. Then,* $Z(G) > Z(G^*)$.

Definition 2. *Assume that* H, X *and* Y *are three connected graphs. And assume that* u, v *are two vertices of* H, v' *is a vertex of* X *and* u' *is a vertex of* Y. *Suppose that* G *is the graph obtained from* H, X, Y *by splicing* v *with* v' *and* u *with* u', *respectively. Assume that* G_1^* *is the graph obtained from* H, X *and* Y *by splicing vertices* v, v' *and* u'. *And suppose that* G_2^* *is the graph obtained from*

H, X and Y by splicing vertices u, v' and u'; for the resulting graph, see Figure 3. We say the transformation from G to $G_i^*(i = 1, 2)$ in Figure 3 is of type **II**.

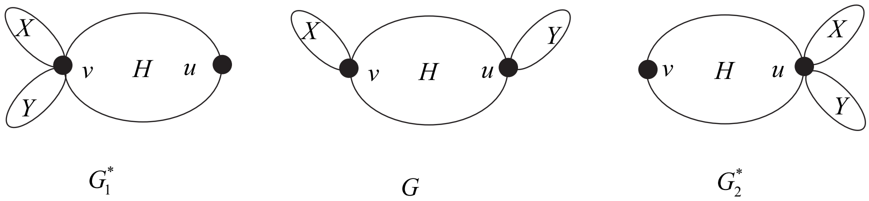

Figure 3. Graphs G, G_1^* and G_2^*.

Lemma 2 ([20])**.** *Assume that G, G_1^* and G_2^* are three graphs of order n defined in Definition 2. Then, $Z(G) > Z(G_1^*)$ and $Z(G) > Z(G_2^*)$.*

Definition 3. *Assume that G is a graph of order $n \geq 7$ obtained from a connected graph $H \neq P_1$ and a cycle $C_q = u_0u_1 \ldots u_{q-1}u_0 (q \geq 4)$ by splicing u_0 with a vertex u of the graph H, see Figure 4. Assume that G^* is a graph obtained from G by a cycle length reduced by one and u_{q-1} is added as a pendant. We say the transformation from G to G^* in Figure 4 is of type* **III**.

Figure 4. Graphs G and G^*.

Lemma 3 ([22])**.** *Suppose that G and G^* are two graphs of order n defined in Definition 3. Then, $Z(G) > Z(G^*)$.*

Definition 4. *Assume that G is a graph of order n obtained by splicing the center of $K_{1,k}$ with a vertex of degree 2 in $B_1(p, q)$; for the resulting graph, see Figure 5. And suppose that G^* is a graph of order n obtained by splicing the center of $K_{1,k}$ with the vertex of degree 4 in $B_1(p, q)$; for the resulting graph, see Figure 5. We say the transformation from G to G^* in Figure 5 is of type* **IV**.

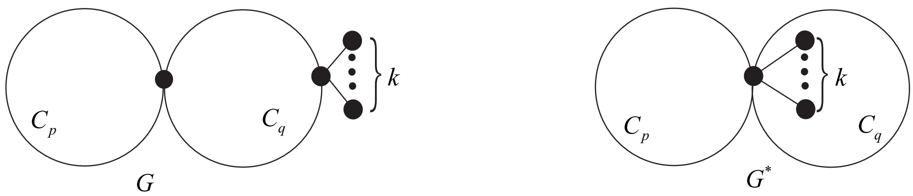

Figure 5. Graphs G and G^*.

Lemma 4 ([23])**.** *Assume that G and G^* are two graphs on n vertices defined in Definition 4. Then, $Z(G) > Z(G^*)$.*

Definition 5. *Assume that G is a graph of order n obtained by splicing the center of $K_{1,k}$ with a vertex of degree 2 in $B_3(p, q, r)$; the resulting graph is shown in Figure 6. And assume that G^* is a graph of order n obtained by splicing the center of $K_{1,k}$ with a vertex of degree 3 in $B_3(p, q, r)$ the resulting graph is shown in Figure 6. We say the transformation from G to G^* in Figure 6 is of type* **V**.

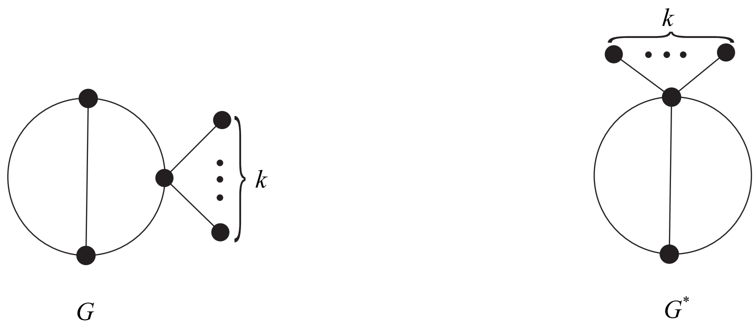

Figure 6. Graphs G and G^*.

Lemma 5 ([20]). *Assume that G and G^* are two graphs of order n defined in Definition 5. Then,* $Z(G) > Z(G^*)$.

Definition 6. *Assume that G is a graph of order n, and assume that* $P_k = x_1x_2\cdots x_k (k \geq 3)$ *is a path in G,* $d_G(x_i) = 2, i = 2, 3, \ldots, k-1$*; the resulting graph is shown in Figure 7. Suppose that* G^* *is a graph of order n obtained from G by deleting* x_2x_3 *and adding* x_1x_3*; the resulting graph is shown in Figure 7. We say the transformation from G to* G^* *in Figure 7 is of type* **VI**.

Figure 7. Graphs G and G^*.

Lemma 6 ([24]). *Suppose that G and G^* are two graphs of order n defined in Definition 6. Then,* $Z(G) > Z(G^*)$.

Finally, we introduce some results which are useful for showing the main theorems later.

Lemma 7 ([18]). *The following identities hold:*
(i) If $G_1, G_2, \ldots, G_r$ *are the connected components of a graph G, then* $Z(G) = \prod_{i=1}^{r} Z(G_i)$.
(ii) If $w \in V(G)$*, then* $Z(G) = Z(G-w) + \sum_{u\in N(w)} Z(G-u-w)$.
(iii) If $e = uw \in E(G)$*, then* $Z(G) = Z(G-e) + Z(G-u-w)$.

Lemma 8 ([10]). *The following identities hold:*
(i) *Assume that G and H are two connected graphs. Then*

$$PS(G \cup H) = PS(G)PS(H).$$

(ii) *Assume that uw is an edge of graph G and* $\mathcal{C}(uw)$ *is the set of cycles containing uw. Then*

$$PS(G) = PS(G-uw) + PS(G-w-u) + 2\sum_{C_k\in\mathcal{C}(uw)} PS(G-V(C_k)).$$

(iii) *Assume that w is a vertex of G and* $\mathcal{C}(w)$ *is the set of cycles containing w. Then*

$$PS(G) = PS(G-w) + \sum_{u\in N_G(w)} PS(G-w-u) + 2\sum_{C_k\in\mathcal{C}(w)} PS(G-V(C_k)).$$

The Fibonacci number $F(t)$ is defined by $F(0) = 0$, $F(1) = 1$ and $F(t) = F(t-1) + F(t-2)$ for $t \geq 2$. Assume that $D(3, n-3)$ is a graph obtained from the disjoint union of a cycle C_3

and a path P_{n-3} by splicing one end of P_{n-3} with one of the vertices of C_3. And assume that S_n^+ is a graph obtained by linking two pendant vertices of star S_n.

Lemma 9 ([10])**.** *Assume that G is a unicyclic graph of order $n(\geq 5)$. Then*

$$2n \leq PS(G) \leq 6F_{n-2} + 2F_{n-3},$$

here the left equality holds if and only if $G \cong S_n^+$, and the right equality holds if and only if $G \cong D(3, n-3)$.

Lemma 10 ([25])**.** *Assume that G is a graph, and $s, t \in V(G)$. And suppose that $G_{p,q}$ is a graph obtained from G by attaching p, q pendent vertices to s and t, respectively. Then*

$$Z(G_{p+i,q-i}) < Z(G_{p,q}) \text{ for } 1 \leq i \leq q; \text{ or } Z(G_{p-i,q+i}) < Z(G_{p,q}) \text{ for } 1 \leq i \leq p.$$

3. The Minimal Hosoya Indices of Bicyclics

Deng [20] considered the Hosoya indices of bicyclic graphs. He characterized a smaller bound of Hosoya indices of bicyclic graphs.

Theorem 2 ([20])**.** *Assume that $G \in \mathscr{B}_n$ is a bicyclic graph of order n. Then*
(i) If $G \in \mathscr{B}_n^1$, then $Z(G) \geq 4n - 8$; here the equality holds if and only if $G \cong B_1^1(3, 3, n-5)$; see Figure 8 for $B_1^1(3, 3, n-5)$.
(ii) If $G \in \mathscr{B}_n^2$, then $Z(G) \geq 8n - 28$; here the equality holds if and only if $G \cong B_2^1(3, 3, 0, n-6)$; see Figure 8 for $B_2^1(3, 3, 0, n-6)$.
(iii) If $G \in \mathscr{B}_n^3$, then $Z(G) \geq 3n - 4$; here the equality holds if and only if $G \cong B_3^1(1, 1, 0, n-4)$; see Figure 8 for $B_3^1(1, 1, 0, n-4)$.
(iv) If $G \in \mathscr{B}_n$, then $Z(G) \geq 3n - 4$; here the equality holds if and only if $G \cong B_3^1(1, 1, 0, n-4)$.

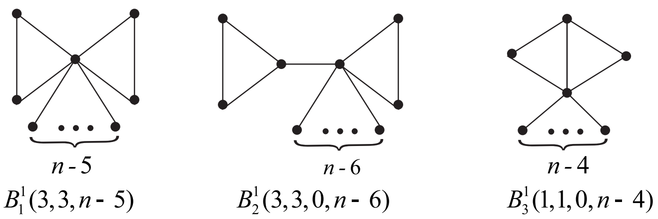

Figure 8. Graphs $B_1^1(3, 3, n-5)$, $B_2^1(3, 3, 0, n-6)$ and $B_3^1(1, 1, 0, n-4)$.

3.1. The Second Minimal Hosoya Index of $G \in \mathscr{B}_n^1$

Lemma 11. *Assume that $G \in \mathscr{B}_n^1 \setminus B_1^1(3, 3, n-5)$ is the graph of order $n \geq 6$. Assume that G has the second minimal Hosoya index. Then, the construct of G is isomorphic to one of the graphs in Figure 9.*

Proof. By Theorem 2 and Lemmas 1–4, there exists the following fact. Assume $G \in \mathscr{B}_n^1 \setminus B_1^1(3, 3, n-5)$ with n vertices. Using multiple transformations **I**, **II**, **III** and **IV** introduced in Definitions 1–4, respectively, the graph G is transformed into $B_1^1(3, 3, n-5)$.That is, there exists graph $G^{(i)}$ for $0 \leq i \leq l$ such that

$$G = G^{(0)} \to G^{(1)} \to G^{(2)} \to \cdots \to G^{(l-1)} \to G^{(l)} = B_1^1(3, 3, n-5), \tag{1}$$

here $G^{(l-1)} \neq B_1^1(3, 3, n-5)$. Now, we determine the construct of $G^{(l-1)}$.

Assume $G \ncong B_1(p, q)$, and suppose that $B_1(s, t)$ denotes the vertex-induced subgraph of G. In the first step, using multiple transformation **I** in Definition 1, all trees of the verticesof $B_1(s, t)$ are turned into stars. This implies that some bicyclic graphs in $\mathscr{B}_n^1$ are changed into $M_1^1(n-5)$, $M_1^2(s, t)$ or $M_1^3(n-6)$. According to the above results, except for all the graphs changed into $M_1^1(n-5)$, $M_1^2(s, t)$ or $M_1^3(n-6)$ in $\mathscr{B}_n^1$, using multiple transformations **II** (resp. **IV**) as in Definition 2 (resp. 4), these graphs are changed into graphs obtained by attaching a star to the common vertex of C_s and C_t in $B_1(s,t)$. Using multiple transformations **III**, these graphs are turned into $B_1^1(3,3,n-5)$. These imply that the construct of $G^{(l-1)}$ is isomorphic to one of $M_1^1(n-5)$, $M_1^2(s,t)$ and $M_1^3(n-6)$. Furthermore, by applying transformation **I** once, G is changed into $B_1^1(3,3,n-5)$. This means that $G^{(l-1)} \cong M_1^4(s,t)$.

Assume $G \cong B_1(p,q)$. Using multiple transformations **III**, these graphs are turned into $B_1^1(3,3,n-5)$. This means that $G^{(l-1)} \cong M_1^3(n-6)$. □

Remark 1. *In fact, by Theorem 2 and Lemmas 1–4, Lemma 11 is obviously valid. The following is what we need to say concerning the process in which every graph in $\mathscr{B}_n^1$ is changed into a graph in Figure 9. The process may apply some graph transformations, and it is difficult to determine which transformation to use first and which to use second.*

Lemma 12. *Each of the following holds.*
(i) If $s \geq 1$, $t \geq 1$ and $s+t+5=n\geq 8$, then $Z(M_1^2(s,t)) \geq 6n-18$, where the equality holds if and only if $M_1^2(s,t) \cong M_1^2(n-6,1)$.
(ii) If $s \geq 1$, $t \geq 0$ and $s+t+5=n\geq 8$, then $Z(M_1^4(s,t)) \geq 8n-28$ with equality holding if and only if $M_1^4(s,t) \cong M_1^4(1,n-7)$.
(iii) $Z(M_1^1(0,n-5)) = 6n-18$ and $Z(M_1^3(n-6)) = 6n-16$.

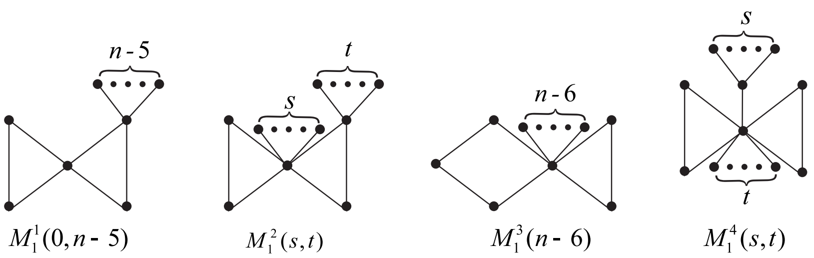

Figure 9. Graphs $M_1^1(0,n-5)$, $M_1^2(s,t)$, $M_1^3(n-6)$ and $M_1^4(s,t)$.

Proof. (i) By Lemma 10, we obtain that $Z(M_1^2(s,t)) \geq Z(M_1^2(n-6,1)) = 6n-18$ or $Z(M_1^2(s,t)) \geq Z(M_1^2(1,n-6)) = 8n-32$. This implies that $Z(M_1^2(s,t)) \geq Z(M_1^2(n-6,1)) = 6n-18$.

(ii) Similarly, by Lemma 10, we obtain that $Z(M_1^4(s,t)) \geq Z(M_1^4(1,n-7)) = 8n-28$ or $Z(M_1^4(s,t)) \geq Z(M_1^4(n-6,0)) = 12n-56$. This means that $Z(M_1^4(s,t)) \geq Z(M_1^4(1,n-7)) = 8n-28$.

(iii) By Lemma 7, a direct computation yields $Z(M_1^1(0,n-5)) = 6n-18$ and $Z(M_1^3(n-6)) = 6n-16$. □

Combining Theorem 2, Lemmas 11 and 12 and (1), it is easy to obtain the second minimal Hosoya index of $G \in \mathscr{B}_n^1$ as follows.

Theorem 3. *Assume that $G \in \mathscr{B}_n^1$ is a bicyclic graph of order $n(\geq 8)$. Then*

$$Z(G) \geq 6n-18 > 4n-8$$

with equality holding if and only if $G \cong M_1^1(0,n-5)$ or $G \cong M_1^2(n-6,1)$.

3.2. The Minimal Hosoya Indices of $G \in \mathscr{B}_n^3$

Similarly, by Theorem 2 and Lemmas 1, 2, 5 and 6, there exists the following fact. Assume $G \in \mathscr{B}_n^3 \setminus B_3^1(1,1,0,n-4)$ on n vertices. With the multiple using transformations **I**, **II**, **V** and **VI**, graph G is transformed into $B_3^1(1,1,0,n-4)$. That is, there exists graph $G^{(i)}$ for $0 \leq i \leq l$ such that

$$G = G^{(0)} \to G^{(1)} \to G^{(2)} \to \cdots \to G^{(l-2)} \to G^{(l-1)} \to G^{(l)} = B_3^1(1,1,0,n-4), \qquad (2)$$

here $G^{(l-1)} \neq B_3^1(1,1,0,n-4)$. According to the above arguments, we can obtain a result that is similar to Lemma 11 as follows.

Lemma 13. *Assume that $G \in \mathscr{B}_n^3 \setminus B_3^1(1,1,0,n-4)$ is the graph of order $n \geq 5$. Assume that G has the second minimal Hosoya index. Then, the construct of G is isomorphic to one of the graphs in Figure 10.*

Proof. The proof is similar to the proof of Lemma 11. Let us omit this proof. □

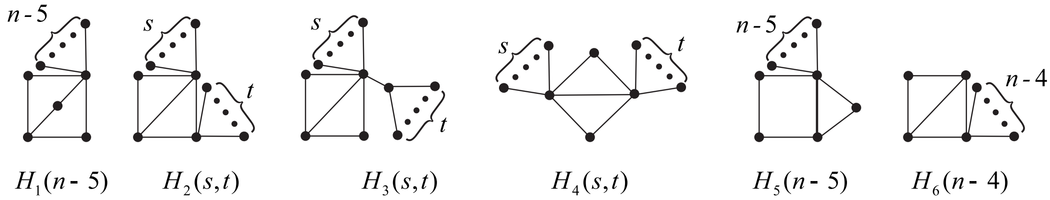

Figure 10. Graphs $H_1(n-5)$, $H_2(s,t)$, $H_3(s,t)$, $H_4(s,t)$, $H_5(n-5)$ and $H_6(n-4)$.

Lemma 14. *Assume that $H_2(s,t)$ is a graph on $n = s+t+4$ vertices. If $n \geq 6, s \geq 1, t \geq 1$ in $H_2(s,t)$, then $Z(H_2(s,t)) \geq 5n-13$ with equality holding if and only if $H_2(s,t) \cong H_2(n-5,1)$.*

Proof. By Lemma 10, we obtain that $Z(H_2(s,t)) \geq Z(H_2(n-5,1)) = 5n-13$ or $Z(H_2(s,t)) \geq Z(H_2(1,n-5)) = 6n-19$. This implies that $Z(H_2(s,t)) \geq Z(H_2(n-5,1)) = 5n-13$. □

Lemma 15. *Suppose that $H_3(s,t)$ is a graph of order $n(= s+t+5)$. If $s \geq 0$, $t \geq 1$ and $n \geq 6$ in $H_3(s,t)$. Then, $Z(H_3(s,t)) \geq 6n-17$ with equality holding if and only if $H_3(s,t) \cong H_3(n-6,1)$.*

Proof. Similarly, by Lemma 10, we obtain that $Z(H_3(s,t)) \geq Z(H_3(n-6,1)) = 6n-17$ or $Z(H_3(s,t)) \geq Z(H_3(0,n-5)) = 8n-29$. This means that $Z(H_3(s,t)) \geq Z(H_3(n-6,1)) = 6n-17$. □

Lemma 16. *Assume that $H_4(s,t)$ is a graph of order $n(\geq 10)$. If $1 \leq s \leq t$, then $4n-9 = Z(H_4(1,n-5)) < 5n-16 = Z(H_4(2,n-6)) < 6n-25 = Z(H_4(3,n-7)) < \cdots Z(H_4(s-1,n-s-5)) < Z(H_4(s,n-s-4))$.*

Proof. By Lemma 7, we obtain that $H_4(s,t) - H_4(s+1,t-1) = t-s+1 > 0$. So $4n-9 = Z(H_4(1,n-5)) < 5n-16 = Z(H_4(2,n-6)) < 6n-25 = Z(H_4(3,n-7)) < \cdots < Z(H_4(s-1,n-s-5)) < Z(H_4(s,n-s-4))$. □

Theorem 4. *Assume $G \in \mathscr{B}_n^3 \setminus B_3^1(1,1,0,n-4)$ on $n \geq 10$ vertices. Then, $Z(G) \geq 4n-9 > 3n-4$ with equality holding if and only if $G \cong H_4(1,n-5)$.*

Proof. By Lemma 7, we obtain that $Z(H_1(n-5)) = 4n-7$, $Z(H_5(n-5)) = 5n-12$ and $Z(H_6(n-4)) = 4n-8$. Combining Theorem 2, Lemmas 13–16, (2) and above arguments, we obtain that $3n-4 < 4n-9 \leq Z(G)$ with the equality holding if and only if $G \cong H_4(1,n-5)$. □

We determine the extremal bicyclic graphs with the third minimal Hosoya index in $\mathscr{B}_n^3$. By (2), it can be known that the extremal bicyclic graphs with the third minimal Hosoya index will be yielded in $G^{(l-1)}$ or $G^{(l-2)}$. By Lemmas 14–16, and the proof of Theorem 4, it can be known that the minimum Hosoya indices in $H_2(s,t)$, $H_3(s,t)$ and $H_5(n-5)$ are more than $5n-16$, respectively. So, we anticipate the third minimal Hosoya index in $\mathscr{B}_n^3$ yields $G^{(l-2)}$ if $G^{(l-1)}$ is $H_1(n-5)$, $H_4(s,t)$ or $H_6(n-4)$. Thus, we determine the lower bounds of the Hosoya indices of $H_1(n-5)$, $H_4(s,t)$ and $H_6(n-4)$ as follows.

Similar to the proof of Lemma 11, by the reverse operations of **I**, **II**, **V** and **VI**, we can obtain that the structures of the graphs $G^{(l-2)}$ if $G^{(l-1)}$ is $H_1(n-5)$, and $G^{(l-2)}$ are isomorphic to one of the graphs $H_1^1(s,t)$, $H_1^2(s,t)$, $H_1^3(s,t)$, $H_1^4(n-6)$ and $H_1^5(n-5)$, see Figure 11.

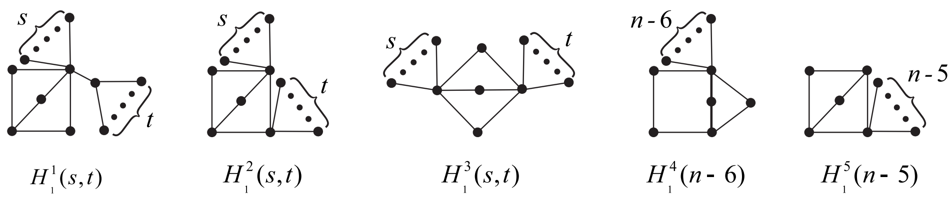

Figure 11. Graphs $H_1^1(s,t)$, $H_1^2(s,t)$, $H_1^3(s,t)$, $H_1^4(n-6)$ and $H_1^5(n-5)$.

Lemma 17. *Assume that $H_1^1(s,t)$ is a graph on $n \geq 7$ vertices. If $s \geq 0$, $t \geq 1$ and $s+t+6=n$, then $Z(H_1^1(s,t)) \geq 8n-26$ with equality holding if and only if $H_1^1(s,t) \cong H_1^1(n-7,1)$.*

Proof. By Lemma 10, we obtain that $Z(H_1^1(s,t)) \geq Z(H_1^1(0,n-6)) = 13n-61$ or $Z(H_1^1(s,t)) \geq Z(H_1^1(n-7,1)) = 8n-26$. This implies that $Z(H_1^1(s,t)) \geq 8n-26$ with equality holding if and only if $H_1^1(s,t) \cong H_1^1(n-7,1)$. □

Lemma 18. *Suppose that $H_1^2(s,t)$ is a graph on $n \geq 7$ vertices. If s and $t \geq 1$ and $s+t+5=n$, then $Z(H_1^2(s,t)) \geq 7n-22$ with equality holding if and only if $H_1^2(s,t) \cong H_1^2(n-6,1)$.*

Proof. By Lemma 10, we know that $Z(H_1^2(s,t)) \geq Z(H_1^2(1,n-6)) = 10n-43$ or $Z(H_1^2(s,t)) \geq Z(H_1^2(n-6,1)) = 7n-22$. This means that $Z(H_1^2(s,t)) \geq 7n-22$ with equality holding if and only if $H_1^2(s,t) \cong H_1^2(n-6,1)$. □

Lemma 19. *Assume that $H_1^3(s,t)$ is a graph of order $n(\geq 7)$. And suppose that $1 \leq t \leq s$ and $s+t+5=n$. Then, $5n-13 \leq Z(H_1^3(s,t))$, where the equality holds if and only if $H_1^3(s,t) \cong H_1^3(n-6,1)$.*

Proof. By Lemma 7, we obtain that $Z(H_1^3(s,t)) - Z(H_1^3(s-1,t+1)) = t-s+1 > 0$. This implies that $5n-13 = Z(H_1^3(1,n-6)) < Z(H_1^3(2,n-7)) < \cdots < Z(H_1^3(s,t))$. □

Theorem 5. *Assume that G is isomorphic to one of the graphs $H_1^1(s,t)$, $H_1^2(s,t)$, $H_1^3(s,t)$, $H_1^4(n-6)$ and $H_1^5(n-5)$. Then, $Z(G) \geq 5n-13$, where the equality holds if and only if $G \cong H_1^3(n-6,1)$.*

Proof. By Lemma 7, we have $Z(H_1^4(n-6)) = 7n-12$ and $Z(H_1^5(n-5)) = 7n-22$. Combining Lemmas 17–19 and above arguments, we obtain that $Z(G) \geq Z(H_1^3(n-6,1)) = 5n-13$. □

Similarly, by the reverse operations of **I**, **II**, **V** and **VI**, we obtain that the construct of graphs $G^{(l-2)}$ if $G^{(l-1)}$ is $H_4(s,t)$, and $G^{(l-2)}$ are isomorphic to one of the graphs $H_4^1(s,t)$, $H_4^2(s,t,u)$, $H_4^3(s,t,u)$, $H_4^4(s,t)$ and $H_4^5(s,t)$, see Figure 12.

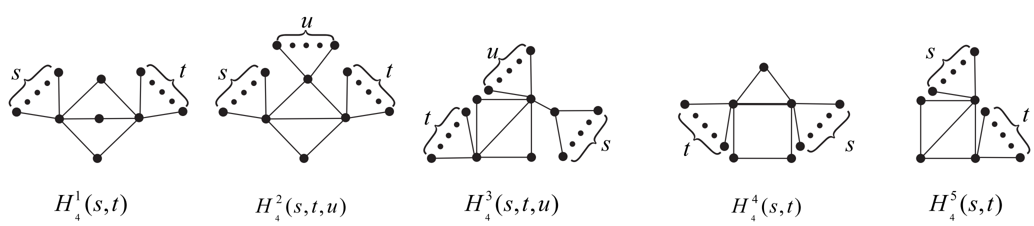

Figure 12. Graphs $H_4^1(s,t)$, $H_4^2(s,t,u)$, $H_4^3(s,t,u)$, $H_4^4(s,t)$ and $H_4^5(s,t)$.

Lemma 20. *Assume that $H_4^2(s,t,u)$ is a graph of order $n(\geq 8)$. If $s+u+t+4=n$, $s \geq 1$, $t \geq 1$ and $u \geq 1$, then $Z(H_4^2(s,t,u)) \geq 7n-25$ with equality holding if and only if $H_4^2(s,t,u) \cong H_4^2(1,n-6,1)$ or $H_4^2(n-6,1,1)$.*

Proof. Assume that two of s, t and u are equal to 1 in $H_4^2(s,t,u)$. By Lemma 7, $Z(H_4^2(1,n-6,1)) = Z(H_4^2(n-6,1,1)) = 7n-25$ and $Z(H_4^2(1,1,n-6)) = 9n-39$. So, $Z(H_4^2(s,t,u)) \geq 7n-25$. Assume that at most one of s, t and u are equal to 1 in $H_4^2(s,t,u)$. By Lemma 7, we obtain that $Z(H_4^2(s,t,u)) = 2n+stu+st+2su+2tu+s+t+2u$. Suppose that $f(s,t,u) = 2n+stu+st+2su+2tu+s+t+2u-(7n-25) = (st-3)u+(2u-4)s+2t(u-2)+st+5$. If $s=1$, $u \geq 2$ and $t \geq 2$, then $f(s,t,u) = (t-1)u+t(2u-3)+1 > 0$. If $t=1$, $u \geq 2$ and $s \geq 2$, then $f(s,t,u) = 3su-(3s+u)+1 > 0$. If $u=1$, $s \geq 2$ and $t \geq 2$, then $f(s,t,u) = 2[st-(s+t)+1] > 0$. Finally, if $s \geq 2$, $t \geq 2$ and $u \geq 2$, then $f(s,t,u) = 2[st-(s+t)+1] > 0$. By the above arguments, we have $Z(H_4^2(s,t,u)) > 7n-25$. □

Lemma 21. *Suppose that $H_4^3(s,t,u)$ is a graph on $n(\geq 8)$ vertices. and assume $s \geq 1$, $t \geq 1$, $u \geq 0$ and $s+u+t+5=n$ in $H_4^3(s,t,u)$. Then, $Z(H_4^3(s,t,u)) \geq 7n-23$ with equality holding if and only if $H_4^3(s,t,u) \cong H_4^3(1,n-6,0)$.*

Proof. Assume that $u=0$, $s \geq 1$ and $t \geq 1$. By Lemma 10, we obtain that $Z(H_4^3(s,t,0)) \geq Z(H_4^3(1,n-6,0)) = 7n-23$ or $Z(H_4^3(s,t,0)) \geq Z(H_4^3(n-6,1,0)) = 11n-51$. This implies that $Z(H_4^3(s,t,0)) \geq 7n-23$. Suppose that $s \geq 1$, $t \geq 1$ and $u \geq 1$. By Lemma 7, we obtain that $Z(H_4^3(s,t,u)-(7n-23) = 6+n+tsu+3su+3ts+tu+7s+3t+2u-(7n-23) = (s-1)(3t+1)+u(ts+3s+t-4) > 0$. This means that $Z(H_4^3(s,t,u)) > 7n-23$. □

Lemma 22. *Suppose that $H_4^4(s,t)$ is a graph on $n(\geq 6)$ vertices. and assume $s \geq 0$, $t \geq 1$ and $s+t+5=n$ in $H_4^4(s,t)$. Then, $Z(H_4^4(s,t)) \geq 5n-12$ with equality holding if and only if $H_4^4(s,t) \cong H_4^4(0,n-5)$.*

Proof. By Lemma 10, we obtain that $Z(H_4^4(s,t)) \geq Z(H_4^4(0,n-5)) = 5n-12$ or $Z(H_4^4(s,t)) \geq Z(H_4^4(n-6,1)) = 7n-24$. This implies that $Z(H_4^4(s,t) \geq 5n-12$, where the equality holds if and only if $H_4^4(s,t) \cong H_4^4(0,n-5)$. □

Checking the constructs of $H_4^1(s,t)$ and $H_4^5(s,t)$, we know that $H_4^1(s,t) \cong H_1^3(s,t)$ and $H_4^5(s,t) \cong H_2(s,t)$. So, combining Lemmas 14 and 19–22, we obtain the following theorem.

Theorem 6. *Assume that G is isomorphic to one of the graphs $H_4^1(s,t)$, $H_4^2(s,t,u)$, $H_4^3(s,t,u)$, $H_4^4(s,t)$ and $H_4^5(s,t)$. Then, $Z(G) \geq 5n-13$, where the equality holds if and only if $G \cong H_1^3(n-6,1)$ or $G \cong H_2(n-5,1)$.*

Similarly, by the reverse operations of **I**, **II**, **V** and **VI**, we can obtain that the structures of the graphs $G^{(l-2)}$ if $G^{(l-2)}$ is $H_6(n-4)$, and $G^{(l-2)}$ are isomorphic to one of the graphs $H_6^1(t,u)$, $H_6^2(t,u)$, $H_6^3(t,u)$ and $H_6^4(n-5)$, see Figure 13.

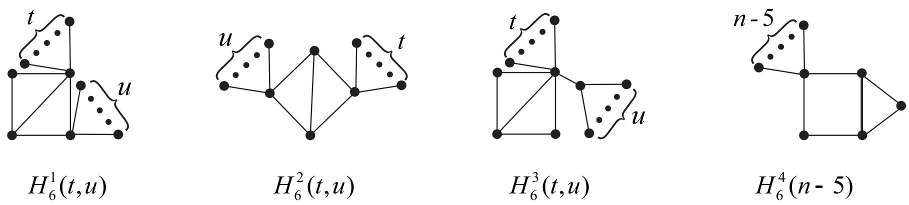

Figure 13. Graphs $H_6^1(t,u)$, $H_6^2(t,u)$, $H_6^3(t,u)$ and $H_6^4(n-5)$.

Lemma 23. *Assume that $H_6^2(t,u)$ is a graph on $n \geq 6$ vertices. Suppose $t \geq u \geq 1$ and $u+t+4=n$ in$H_6^2(t,u)$. Then, $Z(H_6^2(t,u)) \geq 6n-18$ with equality holding if and only if $H_6^2(t,u) \cong H_6^2(n-5,1)$.*

Proof. By Lemma 7, we have $Z(H_6^2(t,u)) - Z(H_6^2(t+1,u-1)) = 2(t+1-u) > 0$. This implies that $6n-18 = Z(H_6^2(n-5,1)) \leq Z(H_6^2(t,u))$. $\square$

Lemma 24. *Assume that $H_6^3(t,u)$ is a graph on $n \geq 7$ vertices. If $t \geq 0$, $u \geq 1$ and $u+t+5=n$, then $Z(H_6^3(t,u)) \geq 8n-28$ with equality holding if and only if $H_6^3(t,u) \cong H_6^3(n-6,1)$ or $H_6^3(t,u) \cong H_6^3(0,n-5)$.*

Proof. By Lemma 10, we obtain that $Z(H_6^3(t,u)) \geq Z(H_6^3(0,n-5)) = 8n-28$ or $Z(H_6^3(s,t)) \geq Z(H_6^3(n-6,1)) = 8n-28$. This means that $Z(H_6^3(t,u)) \geq 8n-28$. $\square$

Theorem 7. *Assume that G is isomorphic to one of the graphs $H_6^1(t,u)$, $H_6^2(t,u)$, $H_6^3(t,u)$ and $H_6^4(n-5,t)$. Then, $Z(G) \geq 5n-13$, and the equality holds if and only if $G \cong H_2(n-5,1)$.*

Proof. Checking graph $H_6^1(t,u)$, we know that $H_6^1(t,u) \cong H_2(s,t)$. By Lemma 7, we obtain that $Z(H_6^4(n-5)) = 6n-17$. Combining Lemmas 14, 23 and 24 and the above argument, we obtain that $Z(G) \geq 5n-13$, where the equality holds if and only if $G \cong H_2(n-5,1)$. $\square$

As mentioned above, the third minimal Hosoya index of G in $\mathscr{B}_n^3$ is yielded in $G^{(l-1)}$ or $G^{(l-2)}$. By the proof of Theorem 4, Theorems 5–7, and Lemmas 14–16, we can obtain the second fifth minimal Hosoya indices of all the graphs in $\mathscr{B}_n^3$. That is,

Theorem 8. *Assume that $G \in \mathscr{B}_n^3$ is a bicyclic graph of order $n(\geq 13)$. Then $Z(G) > 5n-13 = Z(H_1^3(1,n-6)) = Z(H_2(n-5,1)) > 5n-16 = Z(H_4(2,n-6)) > 4n-7 = Z(H_1 (n-5)) > 4n-8 = Z(H_6(n-4)) > 4n-9 = Z(H_4(1,n-5)) > 3n-4 = Z(B_1^1(3,3,0, n-4))$.*

3.3. A Conclusion

Combining Theorems 2, 3 and 8, we can obtain the following results.

Theorem 9. *Assume that $G \in \mathscr{B}_n$ is a bicyclic graph of order $n(\geq 13)$. Then $Z(G) > 5n-13 = Z(H_1^3(1,n-6)) = Z(H_2(n-5,1)) > 5n-16 = Z(H_4(2,n-6)) > 4n-7 = Z(H_1 (n-5)) > 4n-8 = Z(H_6(n-4)) = Z(B_1^1(3,3,n-5)) > 4n-9 = Z(H_4(1,n-5)) > 3n-4 = Z(B_3^1(1,1,0,n-4))$.*

Remark 2. *In this subsection, we provided the second to sixth minimal Hosoya indices of all bicyclic graphs. Using the relevant methods, we can obtain more minimal Hosoya indices in $\mathscr{B}_n$.*

4. The Minimal Permanental Sums of Bicyclic Graphs

In this section, we use the result in Theorem 9 to characterize the second fifth permanental sums in $\mathscr{B}_n$.

Theorem 10 ([21])**.** *Assume that $G \in \mathscr{B}_n = \mathscr{B}_n^1 \cup \mathscr{B}_n^2 \cup \mathscr{B}_n^3$ is a bicyclic graph on $n(n \geq 6)$ vertices.*
(i) If $G \in \mathscr{B}_n^1$, then $PS(G) \geq 4n$; equality holds if and only if $G \cong B_1^1(3,3,n-5)$.
(ii) If $G \in \mathscr{B}_n^3$, then $PS(G) \geq 3n+2$; equality holds if and only if $G \cong B_3^1(1,1,0,n-4)$.
(iii) If $G \in \mathscr{B}_n$, then $PS(G) \geq 3n+2$; equality holds if and only if $G \cong B_3^1(1,1,0,n-4)$.

Theorem 11. *Suppose that $G \in \mathscr{B}_n^1 \setminus B_1^1(3,3,n-5)$ is a bicyclic graph of order $n(\geq 7)$. Then, $PS(G) \geq 6n-8$, where the equality holds if and only if $G \cong M_1^2(n-6,1)$.*

Proof. Assume $G \in \mathscr{B}_n^1 \setminus B_1^1(3,3,n-5)$. By Theorems 1 and 3, and the structures of every graph G in $\mathscr{B}_n^1 \setminus B_1^1(3,3,n-5)$, we obtain that $PS(G) \geq 6n-8$, and the equality holds if and only if G is isomorphic to one of the graphs $M_1^2(n-6,1)$ and $M_1^3(n-6)$. $\square$

Lemma 25. *Assume that $G = S_s^+ \cup S_t^+$ is a graph with $n(= s+t)$ vertices. Then, $PS(G) \geq 12n-3$ with equality holding if and only if $G \cong C_3 \cup S_{n-3}^+$.*

Proof. Without loss of generality, assume $s \leq t$. Suppose that $H = S_{s-1}^+ \cup S_{t+1}^+$. By Lemma 9, we know that $PS(H) - PS(G) = 4(s-1)(1+t) - 4st = 4(s-1-t) < 0$. This implies that the permanental sum of G attains the minimum value when $G = C_3 \cup S_{n-3}^+$, i.e., $PS(G) \geq 12n-3 = PS(C_3 \cup S_{n-3}^+)$. □

Theorem 12. *Assume that $G \in \mathscr{B}_n^2$ is a bicyclic graph of order $n \geq 7$. Then, $PS(G) \geq 12n-32$, and equality holds if and only if $G \cong B_2^1(3,3,0,n-6)$.*

Proof. Suppose that U_s and U_{n-s} are two unicyclic graphs of order s and size $n-s$. Assume that u is a vertex of the cycle in U_s, and suppose that v is a vertex of U_{n-s}. Thus, any graph $G \in \mathscr{B}_n^2$ can be obtained by joining u and v. By Lemma 8, we have

$$PS(G) = PS(G-uv) + PS(G-\{u,v\}) = PS(U_s)PS(U_{n-s}) + PS(U_s-u)PS(U_{n-s}-v). \tag{3}$$

Now we determine the minimum value of $PS(G)$. By (3), $PS(G)$ attains the minimum value if and only if $PS(U_s) \times PS(U_{n-s})$ and $PS(U_s-u) \times PS(U_{n-s}-v)$ obtain the minimum value, respectively. Checking the structure of U_s-u and $U_{n-s}-v$, we know that $PS(U_s-u) \geq 2$ and $PS(U_{n-s}-v) \geq 2$. By Lemmas 8 and 25, we know that $PS(U_s)PS(U_{n-s})$ attains the minimum value only when $U_s \cup U_{n-s} = C_3 \cup S_{n-3}^+$. This implies that G has three possible constructs. That is, G obtained by a vertex of C_3 joining a pendant vertex (or the center, or a vertex of degree 2) of S_{n-s}^+. The graphs are denoted by $B_2^1(3,3,1,n-7)$, $B_2^1(3,3,0,n-6)$ (see Figure 8) and $B_2^2(3,3,0,n-6)$. Direct calculation yields that $PS(B_2^1(3,3,0,n-6)) = 12n-32$, $PS(B_2^2(3,3,0,n-6)) = 14n-44$ and $PS(B_2^1(3,3,1,n-7)) = 16n-52$. Thus, $PS(B_2^1(3,3,0,n-6)) < PS(B_2^2(3,3,0,n-6)) < PS(B_2^1(3,3,1,n-7))$. This completes the proof of Theorem 3. □

Theorem 13. *Assume that $G \in \mathscr{B}_n^3$ is a bicyclic graph on $n \geq 13$ vertices. Then $PS(G) > 5n-7 = PS(H_1^3(n-6,1)) > 5n-10 = PS(H_4(2,n-6)) > 4n-1 = PS(H_1(n-5)) > 4n-3 = PS(H_4(1,n-5)) > 3n+2 = (B_3^1(1,1,0,n-4))$.*

Proof. Suppose that $G \in \mathscr{B}_n^3$. Checking the structures of graphs in $\mathscr{B}_n^3$, and by Lemma 8 and Theorems 1 and 8, we obtain that $PS(H_1^3(n-6,1)) = 5n-7$, $PS(H_4(2,n-6)) = 5n-10$, $PS(H_1(n-5)) = 4n-1$, $PS(H_4(1,n-5)) = 4n-3$, $(B_3^1(1,1,0,n-4)) = 3n+2$, $PS(H_6(n-4)) = 6n-10$ and $PS(H_2(n-5,1)) = 5n-5$. Again by $PS(G) = Z(G) + 2s(G)$, we have $PS(G) > 5n-7 = PS(H_1^3(n-6,1)) > 5n-10 = PS(H_4(2,n-6)) > 4n-1 = PS(H_1(n-5)) > 4n-3 = PS(H_4(1,n-5)) > 3n+2 = (B_3^1(1,1,0,n-4))$. □

Combining Theorems 10–13, we can obtain the second to sixth minimal permanental sums of bicyclic graphs. That is,

Theorem 14. *Assume that $G \in \mathscr{B}_n$ is a bicyclic graph on $n \geq 13$ vertices. Then $PS(G) > 5n-7 = PS(H_1^3(n-6,1)) > 5n-10 = PS(H_4(2,n-6)) > 4n = PS(B_1^1(3,3,n-5)) > 4n-1 = PS(H_1(n-5)) > 4n-3 = PS(H_4(1,n-5)) > 3n+2 = PS(B_3^1(1,1,0,n-4))$.*

5. Conclusions

Wagner and Gutman [18] systematically summarized the research progress of Hosoya indices, and they introduced the applications of Hosoya indices of graphs in chemistry. As an important class of chemical molecular graph, bicyclic graphs have been widely studied for their chemical properties [26–28]. In this article, we determine the second to sixth minimal Hosoya indices among all bicyclic graphs. We use the results to determine the second to sixth minimal permanental sums among all bicyclic graphs. Checking these results, we find that the extremal bicyclic graphs with minimal Hosoya indices and the extremal graphs with minimal permanental sums are different. Furthermore, applying the same method in this article, we can obtain more minimal Hosoya indices and permanental sums among all bicyclic graphs.

Author Contributions: Software, S.X.; Investigation, T.W.; Resources, T.W.; Writing—original draft, T.W.; Writing—review & editing, Y.B. and S.X.; Funding acquisition, T.W. All authors have read and agreed to the published version of the manuscript.

Funding: This article is supported by the National Natural Science Foundation of China (No. 12261071, 11761056) and Natural Science Foundation of Qinghai Province (No. 2020-ZJ-920).

Data Availability Statement: The data presented in this study are available on request from the corresponding author.

Conflicts of Interest: The authors declare no conflicts of interest.

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