On the Hosoya index and the Merrifield-Simmons index of bicyclic graphs with given matching number

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Abstract. Let $\mathscr{B}(n, \alpha)$ be the set of bicyclic graphs on n vertices with matching number α. In this paper, we characterize the extremal bicyclic graph with minimal Hosoya index and maximal Merrifield-Simmons index in $\mathscr{B}(n, \alpha)$.

Keywords: bicyclic graph; matching; independent set

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1. Introduction

Let $G = (V, E)$ denote a simple connected graph with order n and size m. If $m = n - 1 + c$, then G is called a *c-cyclic graph*. If $c = 0, 1$ and 2, then G is a tree, unicyclic graph, and bicyclic graph, respectively.

Two edges of G are said to be independent if they are not adjacent in G. A k-matching of G is a set of k mutually independent edges. We call the number of edges in a maximum matching of G the matching number and denote it by $\alpha(G)$, (or written as α for short). Denote by $z(G)$ the number of matchings in a graph G, that is, $z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} z(G, k)$, where $z(G, k)$ is the number of k-matchings of G for $k \geq 1$ and $z(G, 0) = 1$. Two vertices of G are said to be independent if they are not adjacent in G. An independent k-set is a set of k vertices, no two of which are adjacent. Let $i(G)$ be the number of independent sets of G, then $i(G) = \sum_{k=0}^{n} i(G, k)$, where $i(G, k)$ is the number of k-independent sets of G for $k \geq 1$ and $i(G, 0) = 1$.

The index $z(G)$ (resp. $i(G)$) is also called *Hosoya index*(resp.*Merrifield-Simmons index*) in graphic chemistry. It turned out to be applicable to several questions of molecular chemistry, for example, the connections with physico-chemical properties such as boiling point, entropy or heat of vaporization are well studied [8, 17]. Up to now, many researchers have investigated these graphic invariants. An important direction is to determine

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the graphs with maximal or minimal Hosoya index (or Merrifield-Simmons index, resp.) in a given class of graphs. For instance, it was observed in [9, 14] that the star S_n has the minimal Hosoya index and maximal Merrifield-Simmons index, respectively, and the path P_n has the maximal Hosoya index and minimal Merrifield-Simmons index amongst all trees on n vertices, respectively. Hou [12] characterized the extremal tree with a given matching number respect to Hosoya index. In [22], the present author obtained the extremal unicyclic graph with perfect matching with respect to Hosoya index and Merrifield-Simmons index. Also n-vertex bicyclic graphs have been the object of study of a series of articles by Deng and his coauthors [3, 4, 5, 6]. In particular, Yu and Tian [21] characterized the extremal graphs with minimal Hosoya index and Merrifield-Simmons index, respectively, among all the connected graphs of order n and size $n+t-1$ with $0 \leq t \leq \alpha - 1$. For further details, we refer readers to survey papers [10, 11, 16, 18, 20], especially, a recent paper by S. Wagner and I. Gutman [19], which is a wonderful survey on this topic, and the cited references therein.

2. Preliminaries

Let G be a bicyclic graph, the base of G, denote by $B(G)$, is the minimal bicyclic subgraph of G. Obviously, $B(G)$ is the unique bicyclic subgraph of G containing no pendant vertex, and G can be obtained from $B(G)$ by planting trees to some vertices of $B(G)$. If a tree is attached to a vertex u of $B(G)$, denote it by T_u and call u the root of the tree T_u or the root-vertex of G. It is well known that bicyclic graphs have the following two types of bases: $Q(p,l,q)$ and $P(p,q,r)$, where $Q(p,l,q)$ is the graph obtained by joining a new path $u_1u_2\dots u_l$ between two cycles C_p and C_q with $u_1 \in V(C_p), u_l \in V(C_q)$, and $P(p,q,r)$ is the bicyclic graph consisting of three pairwise internal disjoint paths $P_{p+1}, P_{q+1}, P_{r+1}$ with common endpoints u, v (as shown in Figure 1). Let $\mathscr{B}(n,\alpha)$ be the set of bicyclic graphs on n vertices with matching number α. Let

$$B_1(n) = \{G \in \mathscr{B}(n,\alpha) | B(G) = Q(p,l,q), p \leq q\};$$

$$B_2(n) = \{G \in \mathscr{B}(n,\alpha) | B(G) = P(p,q,r), p \leq q \leq r\}.$$

Then $\mathscr{B}(n,\alpha) = B_1(n) \cup B_2(n)$. In this paper, we characterize the extremal bicyclic graph with minimal Hosoya index and maximal Merrifield-Simmons index in $\mathscr{B}(n,\alpha)$.

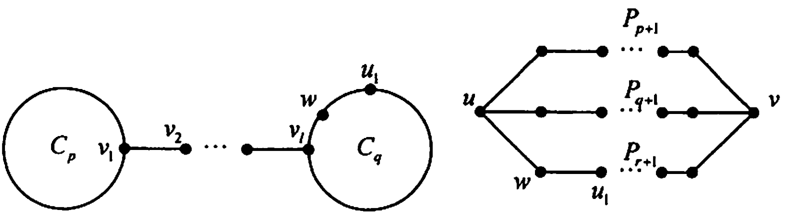

Figure 1: The bases of bicyclic graphs: $Q(p, l, q)$ and $P(p, q, r)$.

In order to state our results, we introduce some notation and terminology. For other undefined notation we refer to Bollobás [1]. For a vertex v of G, denote by $d_G(v)$ the degree of v, $\delta(G)$ the minimum degree of G. Set $N_G(v) = \{u|uv \in E(G)\}$, $N_G[v] = N_G(v) \cup \{v\}$. If $W \subset V(G)$, we denote by $G - W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, if $E \subset E(G)$, we denote by $G - E$ the subgraph of G obtained by deleting the edges of E. If $W = \{v\}$ and $E = \{xy\}$, we write $G - v$ and $G - xy$ instead of $G - \{v\}$ and $G - \{xy\}$, respectively.

Now we give some lemmas that will be used in the proof of our main results.

Lemma 2.1 ([9]). *Let $G = (V, E)$ be a graph.*

(i) *If $uv \in E(G)$, then $z(G) = z(G - uv) + z(G - \{u, v\})$;*
(ii) *If $v \in V(G)$, then $z(G) = z(G - v) + \sum_{u \in N_G(v)} z(G - \{u, v\})$;*
(iii) *If $G_1, G_2, \ldots, G_t$ are the components of the graph G, then $z(G) = \prod_{j=1}^{t} z(G_j)$.*

Lemma 2.2 ([9]). *Let $G = (V, E)$ be a graph.*

(i) *If $uv \in E(G)$, then $i(G) = i(G - uv) - i(G - N_G[u] \cup N_G[v])$;*
(ii) *If $v \in V(G)$, then $i(G) = i(G - v) + i(G - N_G[v])$;*
(iii) *If $G_1, G_2, \ldots, G_t$ are the components of the graph G, then $i(G) = \prod_{j=1}^{t} i(G_j)$.*

From Lemma 2.1 and 2.2, we have

$$z(G) > z(G - uv), \quad z(G) > z(G - v) \tag{2.1}$$

$$i(G) < i(G - uv), \quad i(G) > i(G - v) \tag{2.2}$$

Lemma 2.3 ([15]). *Let H, X, Y be three connected graphs disjoint in pair. Suppose that u, v are two vertices of H, v' is a vertex of X, u' is a vertex of Y. Let G be the graph obtained from H, X, Y by identifying v with v' and u with u', respectively. Let G_1^* be the graph obtained from H, X, Y by identifying vertices v, v', u' and G_2^* be the graph obtained from H, X, Y by identifying vertices u, v', u'. Then*

(i) $z(G_1^*) < z(G)$ *or* $z(G_2^*) < z(G)$;

(ii) $i(G_1^*) > i(G)$ *or* $i(G_2^*) > i(G)$.

Lemma 2.4. *[7] Let G be a graph in $\mathscr{B}(2\alpha, \alpha), \alpha \geq 2$.*

(i) *If $\alpha = 2$, $G \cong P(2,1,2), z(G) = 8, i(G) = 6$;*

(ii) *If $\alpha \geq 3$, $z(G) \geq 4 \cdot 2^{\alpha-1} + (\alpha - 3) \cdot 2^{\alpha-2}$ and $i(G) \leq 2 \cdot 3^{\alpha-1} + 2^{\alpha-3}$, the equalities hold if and only if $G \cong H(2\alpha, \alpha)$, where $H(2\alpha, \alpha)$ is the graph obtained from $Q(3,1,3)$ by attaching a pendent edge and $\alpha - 3$ pendent paths of length 2 at the 4-degree vertex of $Q(3,1,3)$.*

Lemma 2.5. *[13] Let G be a connected graph in the set of unicyclic graphs on n vertices with matching number α and $G \ncong C_n$, where $n > 2\alpha$. Then there are an α-matching M and a pendent vertex v such that M does not saturate v.*

Lemma 2.6. *[1] A matching M in G is a maximum matching if and only if G contains no M-augmenting path.*

3. Main results

In order to prove our main result, we first give two useful lemmas.

Lemma 3.1. *Let G be a graph in $\mathscr{B}(n, \alpha)$,$(n > 2\alpha, \alpha \geq 3)$ and $\delta(G) = 2$, then there exists a graph G' in $\mathscr{B}(n, \alpha)$, satisfying the following three conditions:*

(i) *$\delta(G') = 1$;*

(ii) *there is a α-matching M of G' and a pendent vertex v of G' such that v is M-unsaturated;*

(iii) *$z(G) > z(G')$ and $i(G) < i(G')$.*

Proof. Let G be a graph in $\mathscr{B}(n, \alpha)$ $(n > 2\alpha, \alpha \geq 3)$ and $\delta(G) = 2$, then $G \cong B(G)$. It is easy to see that P_n is a proper spanning subgraph of G. Note that $\alpha \geq \alpha(P_n) = \lfloor \frac{n}{2} \rfloor \geq \alpha$. Hence $n = 2\alpha + 1$. We distinguish two cases as follows.

Case 1. Suppose $G \in B_2(n)$, then $G \cong P(p,q,r)$, where $p \leq q \leq r$ and $p+q+r = n+1$ (as shown in Figure 1).

Let w be the vertex of P_{r+1} adjacent to u, $u_1 (\neq u)$ the vertex adjacent to w on P_{r+1}. Since $n = 2\alpha + 1$ and $\alpha \geq 3$, then $n \geq 7$. Furthermore, $r \geq 3$ and $uu_1 \notin E(G)$. Let $G' = G - u_1 w + uu_1$. It is obvious to see that $P_{2\alpha}$ is a proper subgraph of G', then $\alpha(G') \geq \alpha$. So $G' \in \mathscr{B}(n,\alpha)$. Then G' satisfies (i) and (ii).

Now we prove that G' also satisfies (iii). By Lemma 2.2, we have

$$\begin{aligned} z(G) &= z(G - wu_1) + z(G - w - u_1), \\ z(G') &= z(G' - uu_1) + z(G' - u - u_1); \\ i(G) &= i(G - u_1) + i(G - N_G[u_1]), \\ i(G') &= i(G' - u_1) + i(G' - N_{G'}[u_1]). \end{aligned}$$

Obviously,

$$G - wu_1 \cong G' - uu_1, \qquad G - u_1 \cong G' - u_1.$$

Note that $E(G' - u - u_1)$ is a proper subset of $E(G - w - u_1)$ and $|V(G' - u - u_1)| = |V(G - w - u_1)|$, by (2.1), we have

$$z(G - w - u_1) > z(G' - u - u_1).$$

Let $G' - N_{G'}[u_1] = P_1 \cup A$, where A is the component of $G' - N_{G'}[u_1]$ which isn't containing w. Then

$$\begin{aligned} i(G' - N_{G'}[u_1]) &= 2i(A), \\ i(G - N_G[u_1]) &= i(G - N_G[u_1] - u) + i(G - N_G[u_1] \cup N_{G - N_G[u_1]}[u]) \\ &= i(A) + i(G - N_G[u_1] \cup N_{G - N_G[u_1]}[u]), \end{aligned}$$

and $V(G - N_G[u_1] \cup N_{G - N_G[u_1]}[u])$ is a proper subset of $G - N_G[u_1] - u$, by (2.2), we have

$$i(A) > i(G - N_G[u_1] \cup N_{G - N_G[u_1]}[u]),$$

then

$$i(G - N_G[u_1]) < i(G' - N_{G'}[u_1]).$$

Hence $z(G) > z(G')$ and $i(G) < i(G')$.

Case 2. Suppose $G \in B_1(n)$, then $G \cong Q(p,l,q)$, where $p \leq q$ (as shown in Figure 1).

(a) If $l = 1$, then $p + q = n + 1$. Then $q \geq 4$. Let $G' = G - u_1w + v_lu_1$.
(b) If $l \geq 2$ and $q \geq 4$. Let $G' = G - u_1w + v_lu_1$.
(c) If $l \geq 2$ and $p = q = 3$. Let $G' = G - v_2v_3 + v_1v_3$.

Similar to the discussion of case 1, we can prove that G' satisfies (i), (ii) and (iii). □

Lemma 3.2. *Let G be a graph in $\mathscr{B}(n, \alpha)$ $(n > 2\alpha, \alpha \geq 3)$ and $\delta(G) = 1$, then there is an α-matching M of G and a pendent vertex v of G such that v is M-unsaturated; or there exists a graph G' in $\mathscr{B}(n, \alpha)$, satisfying the following two conditions:*

(i) *$z(G) > z(G')$ and $i(G) < i(G')$;*
(ii) *there is an α-matching M of G' and a pendent vertex v of G' such that v is M-unsaturated.*

Proof. Let G be a graph in $\mathscr{B}(n, \alpha)$ $(n > 2\alpha)$ with $\delta(G) = 1$ and M be an α-matching of G. If there is a pendent vertex v of G such that v is M-unsaturated, the result holds immediately. So we suppose each pendent vertex of G is M-saturated.

Let $B(G)$ be the base of G, then $\delta(B(G)) = 2$. Let u be a vertex of $B(G)$ with $d_{B(G)}(u) \geq 3$, then u must be a vertex of a cycle, denote it by $C_{B(G)}$, in $B(G)$. Among two edges in $E(C_{B(G)})$ incident with u, there must be one edge belonging to $E(G) \setminus M$. we denote this edge by uu_1, then $G - uu_1$ is a n-vertex unicyclic graph with an α-matching M. Then $\alpha(G - uu_1) \geq \alpha$. Note that $G - uu_1 \subset G$, we have $\alpha(G - uu_1) \leq \alpha(G) = \alpha$. So $\alpha(G - uu_1) = \alpha$. By Lemma 2.5, there are an α-matching M' of $G - uu_1$ and a pendent vertex v' of $G - uu_1$ such that v' is M'-unsaturated.

If $v' \neq u_1$, then v' is also a pendent vertex of G. Noting that M' is also an α-matching of G. Then G and M' satisfy the requirements.

If $v' = u_1$, we distinguish the following two cases.

Case 1. There exists a vertex v'' of some tree T_w such that v'' is M'-unsaturated.

If v'' is a pendent vertex of G, then G and M' satisfy the requirements.

If v'' isn't a pendent vertex of G, we can find a maximal M'-alternating path P which stars from v'' and terminates at a pendent vertex v of G. By Lemma 2.6, we know that v is M'-saturated. Then the symmetric difference $M' \oplus P$ is an α-matching of G. Then G and $M' \oplus P$ satisfy the requirements.

Case 2. For any root-vertex w of G, each vertex of T_w is M'-saturated.

Let u_2 be the unique vertex of $B(G) - uu_1$ adjacent to u_1, obviously u_2 must be M'-saturated. We can construct a maximal M'-alternating path $P = u_1u_2 \dots u_{2t}u_{2t+1}$ of $G - uu_1$, obeying the following principal:

> For each j $(1 \le j \le t)$, if $u_{2j}, u_{2j+1} \in V(B(G))$ and $N_G(u_{2j+1}) \setminus B(G) \neq \emptyset$, we choose a vertex from $N_G(u_{2j+1}) \setminus B(G)$ as u_{2j+2}.

By Lemma 2.6, we know that u_{2t+1} is M'-saturated.

If u_{2t+1} is a pendent vertex of G, then G and $M' \oplus P$ satisfy the requirements.

Otherwise, P is a spanning subgraph of $B(G)$. Then u_1 is the unique M'-unsaturated vertex of G and u_{2j+1} $(1 \le j \le t)$ is not the root-vertex of G. Note that the order of P is odd, that is, the order of $B(G)$ is odd.

If $B(G) \ncong B(3,1,3)$, we can choose an appropriate vertex u_{2j+1} $(0 \le j \le t)$ and get a graph $G' = G - u_{2j+1}u_{2j+2} + u_{2j}u_{2j+2}$. Noting that $u_{2j+1}u_{2j+2} \notin M'$, M' is also an α-matching of G', then $G' \in \mathscr{B}(n, \alpha)$. Furthermore,

$$\begin{aligned}
z(G) &= z(G - u_{2j+1}u_{2j+2}) + z(G - u_{2j+1} - u_{2j+2}),\\
z(G') &= z(G' - u_{2j}u_{2j+2}) + z(G' - u_{2j} - u_{2j+2});\\
i(G) &= i(G - u_{2j+1}) + i(G - N_G[u_{2j+1}]),\\
i(G') &= i(G' - u_{2j+1}) + i(G' - N_{G'}[u_{2j+1}]).
\end{aligned}$$

Note that

$$\begin{aligned}
G - u_{2j+1}u_{2j+2} \cong G' - u_{2j}u_{2j+2}, &\quad G' - u_{2j} - u_{2j+2} \subset G - u_{2j+1} - u_{2j+2},\\
G - u_{2j+1} \cong G' - u_{2j+1}, &\quad G - N_G[u_{2j+1}] \subset G' - N_{G'}[u_{2j+1}],
\end{aligned}$$

and

$$\begin{aligned}
& i(G' - N_{G'}[u_{2j+1}])\\
= & \; i(G' - N_{G'}[u_{2j+1}] - u_{2j}) + i(G' - N_{G'}[u_{2j+1}] \cup N_{G' - N_{G'}[u_{2j+1}]}[u_{2j}])\\
= & \; i(G - N_G[u_{2j+1}]) + i(G' - N_{G'}[u_{2j+1}] \cup N_{G' - N_{G'}[u_{2j+1}]}[u_{2j}])\\
> & \; i(G - N_G[u_{2j+1}]).
\end{aligned}$$

Then $z(G) > z(G')$ and $i(G) < i(G')$. Let $P' = u_1u_2 \dots u_{2j}u_{2j+1}$ $(0 \le j \le t)$, obviously u_{2j+1} is $M' \oplus P'$-unsaturated. Then G' and $M' \oplus P'$ satisfy the requirements.

If $B(G) \cong Q(3,1,3)$, it is easy to get an α-matching M'' and an M''-unsaturated pendent vertex. Then G and M'' satisfy the requirements.

This completes the proof. $\square$

Let $H(n,\alpha)$ be the graph obtained from $Q(3,1,3)$ by attaching $n-2\alpha+1$ pendent edges and $\alpha-3$ pendent paths of length 2 at the 4-degree vertex of $Q(3,1,3)$ (as shown in Figure 2). For convenience, let u' be the unique 4-degree vertex in $Q(3,1,3)$ and v' be a pendent vertex which is adjacent to u' in $H(n,\alpha)$.

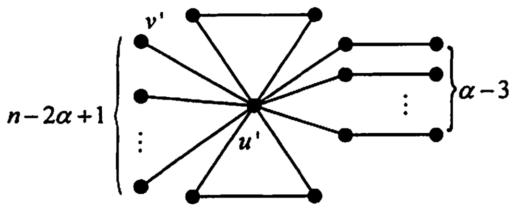

Figure 2: The graph $H(n,\alpha)$.

Theorem 3.3. *Let G be a graph in $\mathscr{B}(n,\alpha)$ $(n>2\alpha,\alpha\geq 3)$, then $z(G)\geq (n-2\alpha+4)\cdot 2^{\alpha-1}+(\alpha-3)\cdot 2^{\alpha-2}$ and $i(G)\leq 3^{\alpha-1}\cdot 2^{n-2\alpha+1}+2^{\alpha-3}$. The equalities hold if and only if $G\cong H(n,\alpha)$.*

Proof. Let G be a graph in $\mathscr{B}(n,\alpha)$ $(n>2\alpha,\alpha\geq 3)$ and $G\ncong H(n,\alpha)$. We prove the results by induction on n.

If $n=2\alpha$, the results hold by Lemma 2.4.

Now we suppose $n>2\alpha$ and the results hold for all the graphs in $\mathscr{B}(n-1,\alpha)$ which are not isomorphic to $H(n-1,\alpha)$. By lemmas 3.1 and 3.2, we can distinguish two cases as follows.

(a) There is a maximum matching M of G and a pendent vertex v of G such that v is M-unsaturated. Let u be the vertex of G adjacent to v. By Lemma 2.1 and Lemma 2.2, we have

$$\begin{aligned}
z(G) &= z(G-uv)+z(G-u-v)\\
&= z(G-v)+z(G-u-v),\\
z(H(n,\alpha)) &= z(H(n,\alpha)-u'v')+z(H(n,\alpha)-u'-v')\\
&= z(H(n,\alpha)-v')+z(H(n,\alpha)-u'-v');\\
i(G) &= i(G-v)+i(G-N_G[v])\\
&= i(G-v)+i(G-u-v),\\
i(H(n,\alpha)) &= i(H(n,\alpha)-v')+i(H(n,\alpha)-N_{G'}[v'])\\
&= i(H(n,\alpha)-v')+i(H(n,\alpha)-u'-v').
\end{aligned}$$

It is easy to see that $G - v \in \mathscr{B}(n-1, \alpha)$ and $H(n, \alpha) - v' \cong H(n-1, \alpha)$. By the induction hypothesis, we have

$$z(G - v) > z(H(n, \alpha) - v') \quad \textit{and} \quad i(G - v) < i(H(n, \alpha) - v').$$

Note that

$$H(n, \alpha) - u' - v' \cong (\alpha - 1)K_2 \cup (n - 2\alpha)K_1,$$

$G \not\cong H(n, \alpha)$, and $G - u - v$ has an $(\alpha - 1)$-matching, then $H(n, \alpha) - u' - v'$ is a proper spanning subgraph of $G - u - v$. Then

$$\begin{aligned} z(G - u - v) &> z(H(n, \alpha) - u' - v') \\ i(G - u - v) &< i(H(n, \alpha) - u' - v'). \end{aligned}$$

Hence $z(G) > z(H(n, \alpha))$ and $i(G) < i(H(n, \alpha))$.

(b) If there exists a graph G' in $\mathscr{B}(n, \alpha)$, satisfying the following two conditions:

(i) $z(G) > z(G')$ and $i(G) < i(G')$;
(ii) there is a maximum matching M of G' and a pendent vertex v of G' such that v is M-unsaturated.

Similar to (a), we can obtain $z(G') > z(H(n, \alpha))$ and $i(G') < i(H(n, \alpha))$.
By Lemma 2.1 and Lemma 2.2, we have

$$\begin{aligned} z(H(n, \alpha)) &= z(H(n, \alpha) - u') + \sum_{x \in N_{H(n,\alpha)}(u')} z(H(n, \alpha) - u' - x) \\ &= (n - 2\alpha + 4) \cdot 2^{\alpha - 1} + (\alpha - 3) \cdot 2^{\alpha - 2}; \\ i(H(n, \alpha)) &= z(H(n, \alpha) - u') + i(H(n, \alpha) - N_{H(n,\alpha)}[u']) \\ &= 3^{\alpha - 1} \cdot 2^{n - 2\alpha + 1} + 2^{\alpha - 3}. \end{aligned}$$

Then we obtain the desirable results. □

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