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On the harmonic index of bicyclic conjugated molecular graphs

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Abstract. The harmonic index $H(G)$ of a graph G is defined as the sum of weights $\frac{2}{d(u)+d(v)}$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G. In this paper, we first present a sharp lower bound on the harmonic index of bicyclic conjugated molecular graphs (bicyclic graphs with perfect matching). Also a sharp lower bound on the harmonic index of bicyclic graphs is given in terms of the order and given size of matching.

1. Introduction

We first introduce some terminologies and notations of graphs. Undefined terminologies and notations may refer to [1]. We only consider finite, undirected and simple graphs. Denote by C_n the cycle of n vertices. Unicyclic graphs are connected graphs with n vertices and n edges. For a vertex x of a graph G, we denote the neighborhood and the degree of x by $N(x)$ and $d(x)$, respectively. A pendant vertex is a vertex of degree 1. Denote by PV the set of pendant vertices of G. Let $d_G(x, y)$ denote the length of a shortest (x, y)-path in G. We will use $G - x$ to denote the graph that arises from G by deleting the vertex $x \in V(G)$ together with its incident edges. A subset $M \subseteq E$ is called a *matching* in G if its elements are edges and no two are adjacent in G. A matching M saturates a vertex v, and v is said to be M-saturated, if some edges of M is incident with v. If every vertex of G is M-saturated, the matching M is *perfect*. A matching M is said to be an *m-matching* (or a *maximum matching*), if $|M| = m$ and for every matching M' in G, $|M'| \leq m$.

The Randić index of an organic molecule whose molecular graph is G was introduced by the chemist Milan Randić in 1975 [8] as

$$R(G) = \sum_{uv} \frac{1}{\sqrt{d(u)d(v)}},$$

where $d(u)$ and $d(v)$ stand for the degrees of the vertices u and v, respectively, and the summation goes over all edges uv of G. Recently, finding bounds for the Randić index of a given class of graphs, as well as related

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problem of finding the graphs with extremal Randić index, attracted the attention of many researchers, and many results have been obtained (see recent books [4] and [6]).

In this paper, we consider another variant of the Randić index, named the harmonic index. For a graph G, the harmonic index $H(G)$ is defined (see [2]) as

$$H(G) = \sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}.$$

In [3], the authors considered the relation between the harmonic index and the eigenvalues of graphs. In [10], [11] and [12], the authors presented the minimum and maximum values of harmonic index on simple connected graphs, trees, unicyclic graphs and bicyclic graphs respectively. In [5] and [9], the authors established some relationships between harmonic index and several other topological indices, such as the Zagreb index and the atom-bond connectivity index.

Bicyclic graphs are connected graphs in which the number of edges equals the number of vertices plus one. The bicyclic graphs of order n without pendant vertex are characterized as follows:

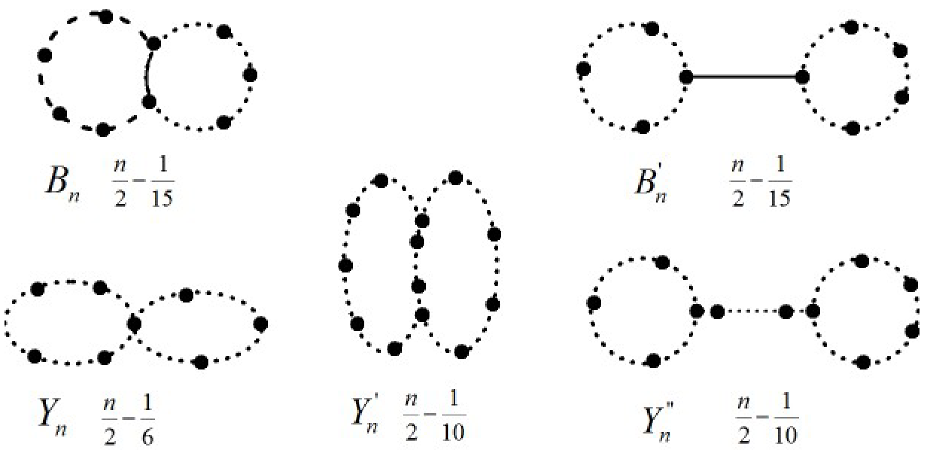

Figure 1 Bicyclic graphs without pendant vertex and their harmonic indices.

Let n and m be positive integers with $n \geq 2m$. Let $U_{n,m}$ be a graph with n vertices obtained from C_3 by attaching $n-2m+1$ pendant edges and $m-2$ paths of length 2 to one vertex of C_3. Let $B_{n,m}$ be a graph with n vertices obtained from Y_5 by attaching $n-2m+1$ pendant edges and $m-3$ paths of length 2 to the unique vertex of degree four in Y_5 (see Figure 2). Denote $\mathscr{U}_{n,m}$={G: G is a unicyclic graph with n vertices and an m-matching}, $\mathscr{B}_{n,m}$={G: G is a bicyclic graph with n vertices and an m-matching}.

Researchers are interested in the extremal graph theory for a type of graphs, i.e., the connected graphs with perfect matchings. In this paper, we first present a sharp lower bound on the harmonic index of bicyclic conjugated molecular graphs (bicyclic graphs with a perfect matching). Also a sharp lower bound on the harmonic index of bicyclic graphs is given in terms of the order and given size of matching.

2. Some lemmas

Lemma 2.1. *[7] Let $G \in \mathscr{B}_{2m,m}$. If $PV \neq \phi$, then for any vertex $u \in V(G)$, $|N(u) \cap PV| \leq 1$.*

Lemma 2.2. *[14] Let $G \in \mathscr{B}_{2m,m}$, $m \geq 3$, and let T be a tree in G attached to a root r. If $v \in V(T)$ is a vertex furthest from the root r with $d_G(v,r) \geq 2$, then v is a pendant vertex and adjacent to a vertex u of degree 2.*

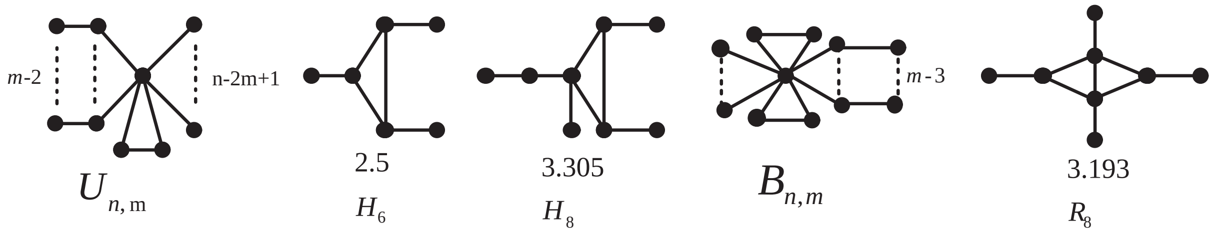

Figure 2

Lemma 2.3. *[14] Let $G \in \mathscr{B}_{n,m}(n > 2m)$ and G has at least one pendant vertex. Then there is an m-matching M and a pendant vertex v such that M does not saturate v.*

Lemma 2.4. *[13] Let x, y be positive integers with $1 \le x \le y-1$. Denote $\kappa(x,y) = \frac{2x+2}{y+1} + \frac{2(y-x-1)}{y+2}$. Then the function $\kappa(x-1,y) - \kappa(x,y+1)$ are monotonously increasing in $x \ge 1$ and $y \ge 0$, respectively.*

3. Main Results

Let n and m be positive integers with $n \ge 2m$. Let $U_{n,m}$ be a graph with n vertices obtained from C_3 by attaching $n-2m+1$ pendant edges and $m-2$ paths of length 2 to one vertex of C_3 (see Figure 2). Denote $\varphi(n,m) = \frac{2(m-2)}{3} + \frac{2m}{n-m+3} + \frac{2(n-2m+1)}{n-m+2} + \frac{1}{2}$.

Theorem 3.1. *[13] Let $G \in \mathscr{U}_{2m,m} \backslash \{H_6, H_8\}$ $(m \ge 2)$. Then*

$$H(G) \ge \varphi(2m, m),$$

with equality holds if and only if $G \cong U_{2m,m}$ (see Figure 2).

Theorem 3.2. *[12] Among connected bicyclic graphs on n vertices, $n \ge 4$, the graph of the type B_n and B'_n have maximum harmonic index, and $H(B_n) = H(B'_n) = \frac{n}{2} - \frac{1}{15}$ (see Figure 1).*

Denote $\psi(n,m) = \frac{2(n-2m+1)}{n-m+3} + \frac{2m+2}{n-m+4} + \frac{2m}{3} - 1$, where n and m are positive integers and $n \ge 2m$.

Theorem 3.3. *Let $G \in \mathscr{B}_{2m,m} \backslash \{R_8\}$ $(m \ge 3)$. Then $H(G) \ge \psi(2m,m)$, with equality holds if and only if $G \cong B_{2m,m}$ (see Figure 2).*

Proof. First we note that if $G \cong B_{2m,m}$, then $H(G) = \psi(2m,m)$. We apply induction on m.

Now we prove that if $G \in \mathscr{B}_{2m,m} \backslash \{R_8\}$, then the result holds. If $m = 3$, $\psi(6,3) = 2.476$, note that the total 17 graphs with their harmonic indices are listed in Figure 3. Thus the theorem holds for $m = 3$.

We now suppose that $m \ge 4$ and proceed by induction on m.

If G has no pendant vertex, then G is one of the type of $\{B_{2m}, B'_{2m}, Y_{2m}, Y'_{2m}, Y''_{2m}\}$. It is easy to prove that $\min\{H(B_{2m}), H(B'_{2m}), H(Y_{2m}), H(Y'_{2m}), H(Y''_{2m})\} = H(Y_{2m}) = m - \frac{1}{6} > \psi(2m,m)$. Hence, now we assume that G has at least one pendant vertex.

By Lemmas 2.1 and 2.2, we only consider the following two cases.

Case 1. G has a pendant vertex v which is adjacent to a vertex w of degree 2.

In this case, there is a unique vertex $u \ne v$ such that $uw \in E(G)$. Denote $d(u) = t$ and $N(u) = \{w, y_1, \dots, y_{t-1}\}$, then $t \ge 2$. Since G is a bicyclic graph with a perfect matching, then $t \le m+2$. By Lemma 2.1, there exists at most one vertex in $\{y_i\}$ $(i = 1, 2, \dots, t-1)$ has degree one, say $i = 1$, such that $d(y_1) \ge 1$, the degree of other vertices are at least two. Let $G' = G - v - w$. Then $G' \in \mathscr{B}_{2m-2,m-1}$.

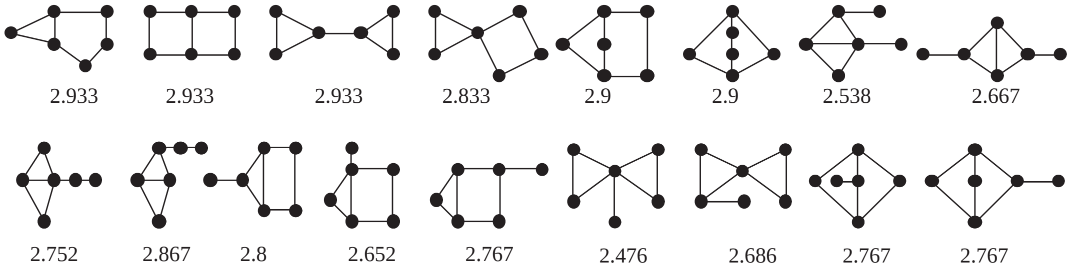

Figure 3

If $G' \cong R_8$, then $G \in \{G_i | 1 \leq i \leq 4\}$, where $G_i(1 \leq i \leq 4)$ and their harmonic indices are illustrated in Figure 4. By $\psi(10, 5) = 3.917$, it is easy to verify that $B_{10,5}$ has the minimum harmonic indices among all bicyclic graphs in $\{G_i | 1 \leq i \leq 4\} \cup \{B_{10,5}\}$.

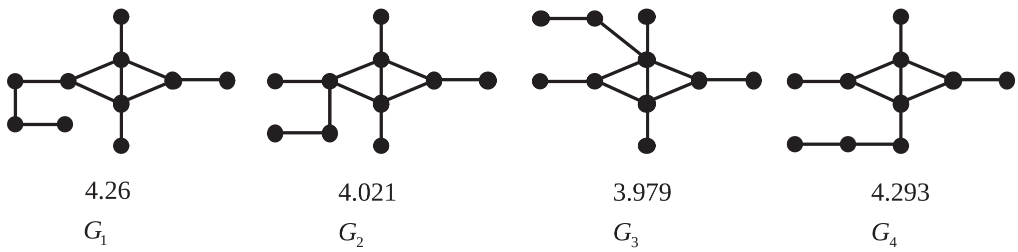

Figure 4

Otherwise, if $G' \ncong R_8$, by the induction hypothesis, then

$$
\begin{aligned}
H(G) &= H(G') + \frac{2}{3} + \frac{2}{t+2} + \sum_{i=1}^{t-1} \frac{2}{t+d(y_i)} - \sum_{i=1}^{t-1} \frac{2}{t+d(y_i)-1} \\
&\geq \psi(2m-2, m-1) + \frac{2}{3} + \frac{2}{t+2} - \frac{2}{t(t+1)} - \frac{2(t-2)}{(t+1)(t+2)} \\
&= \psi(2m-2, m-1) + \frac{2}{3} + \frac{4t-4}{t(t+1)(t+2)}.
\end{aligned}
$$

Since $\frac{4t-4}{t(t+1)(t+2)}$ is strictly monotonously decreasing in t and $t \leq m+2$, we have

$$
H(G) \geq \psi(2m, m) + \frac{2}{m+2} - \frac{8}{m+3} + \frac{6}{m+4} + \frac{4m+4}{(m+2)(m+3)(m+4)} = \psi(2m, m).
$$

The equality $H(G) = \psi(2m, m)$ holds if and only if equality holds throughout the above inequalities, that is if and only if $G' \cong B_{2m-2,m-1}$, $d(y_1) = 1$, $d(y_i) = 2$ for $i = 2, 3, \ldots, t-1$ and $t = m+2$. Thus $G \cong B_{2m,m}$.

Case 2. G is one of the type of $\{B_s, B_s', Y_s, Y_s', Y_s''\}$ $(4 \leq s < 2m)$ attached by some pendant edges.

If there is no vertex of degree two, then $G \in \{F_i | 1 \leq i \leq 7\}$, where $F_i(1 \leq i \leq 7)$ is illustrated in Figure 5. In F_1, if $m = 4$, then $H(F_1) = 3.5 > \psi(8, 4) = 3.202$. In F_2, we have $m \geq 5$ because $G \ncong R_8$. If $m = 5$, then $H(F_2) = 4.026 > \psi(10, 5) = 3.917$. In F_3, if $m = 5$, then $H(F_3) = 4.333 > \psi(10, 5) = 3.917$. In F_4, if $m = 6$, then

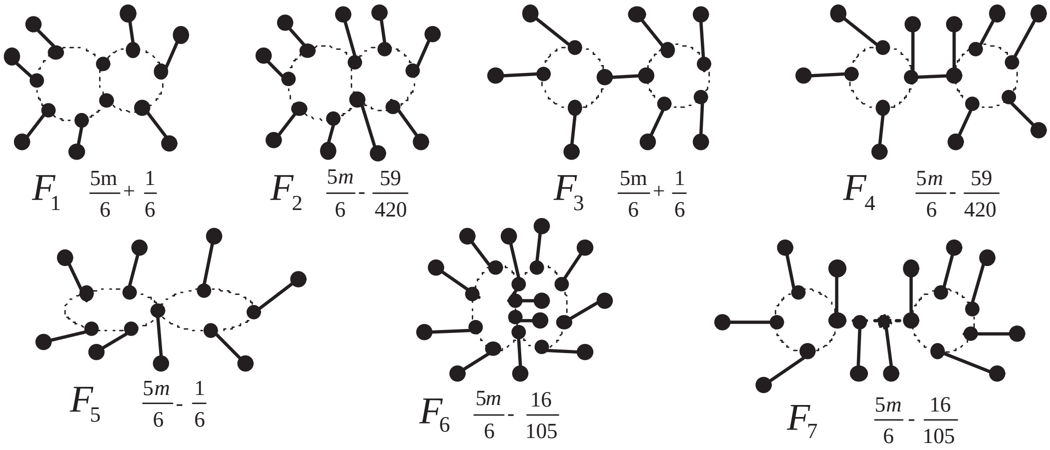

Figure 5

$H(F_4) = 4.86 > \psi(12,6) = 4.622$. In F_5, if $m = 5$, then $H(F_5) = 4 > \psi(10,5) = 3.917$. In F_6, if $m = 5$, then $H(F_6) = 4.014 > \psi(10,5) = 3.917$. In F_7, if $m = 7$, then $H(F_7) = 5.681 > \psi(14,7) = 5.321$. We can clearly see that the harmonic index of each $F_i (1 \le i \le 7)$ can be expressed by the form of $H(F_i) = \frac{5m}{6} + c_i$, where c_i is a constant $(1 \le i \le 7)$. By the induction hypothesis, then

$$\begin{aligned}
H(F_i) &= \frac{5(m-1)}{6} + c_i + \frac{5}{6} \ge \psi(2m-2, m-1) + \frac{5}{6} \\
&= \psi(2m, m) + \frac{2}{m+2} - \frac{8}{m+3} + \frac{6}{m+4} + \frac{1}{6} \\
&> \psi(2m, m) + \frac{2}{m+3} - \frac{2}{m+3} - \frac{6}{m+3} + \frac{6}{m+4} + \frac{1}{6} \\
&= \psi(2m, m) + \frac{(m+\frac{7}{2})^2 - \frac{145}{4}}{6(m+3)(m+4)} > \psi(2m, m),
\end{aligned}$$

where the last inequality holds since $m \ge 4$.

Otherwise, there is at least a vertex of degree two on G. We assume that $d(u) = 2$, v and w are the two vertices adjacent to u.

Subcase 2.1. The vertex u is on one of the two cycles of G.

By the definition of matching, among the edges adjacent to u, there is a unique edge uw (or uv) which not belong to the m-matching, without loss of generality, denote it by uw. Denote $d(w) = t, N(w)\backslash\{u\} = \{x_1, x_2, \ldots, x_{t-1}\}$. We have $2 \le t \le 5$, $2 \le d(v) \le 5$, $d(x_i) \ge 1$ $(1 \le i \le t-1)$. By Lemma 2.1, there is at most one vertex in $\{x_1, x_2, \ldots, x_{t-1}\}$ which is degree 1. Let $G' = G - uw$. Obviously, we have $G' \in \mathscr{U}_{2m,m}$. Since $m \ge 4$, by Theorem 3.1, if $G' \ncong H_8$, we have

$$\begin{aligned} H(G) &= H(G') + \frac{2}{2+d(v)} - \frac{2}{1+d(v)} + \frac{2}{t+2} + \sum_{i=1}^{t-1} \frac{2}{t+d(x_i)} - \sum_{i=1}^{t-1} \frac{2}{t+d(x_i)-1} \\ &= H(G') - \frac{2}{(1+d(v))(2+d(v))} + \frac{2}{t+2} - \sum_{i=1}^{t-1} \frac{2}{(t+d(x_i))(t+d(x_i)-1)} \\ &\geq H(G') - \frac{2}{3\times 4} + \frac{2}{t+2} - \frac{2(t-1)}{t(t+1)} \\ &\geq \frac{2m}{3} + \frac{2m}{m+3} + \frac{2}{m+2} - 1 + \frac{t^3-t^2-2t+4}{t(t+1)(t+2)}. \end{aligned}$$

Since $\frac{t^3-t^2-2t+4}{t(t+1)(t+2)}$ is strictly monotonously increasing in t and $m \geq 4$, $2 \leq t \leq 5$, we have

$$\begin{aligned} H(G) - \psi(2m, m) &\geq \frac{2m}{3} + \frac{2m}{m+3} + \frac{2}{m+2} - 1 + \frac{1}{6} - \psi(2m, m) \\ &= \frac{2}{m+2} - \frac{8}{m+3} + \frac{6}{m+4} + \frac{1}{6} \\ &> \frac{(m+\frac{7}{2})^2 - \frac{145}{4}}{6(m+3)(m+4)} > 0. \end{aligned}$$

If $G' \cong H_8$, then $G \in \{Q_i | 1 \leq i \leq 11\}$ since $G \ncong R_8$, where $Q_i (1 \leq i \leq 11)$ are illustrated in Figure 6. Thus $H(Q_i) > \psi(8, 4) = 3.202$.

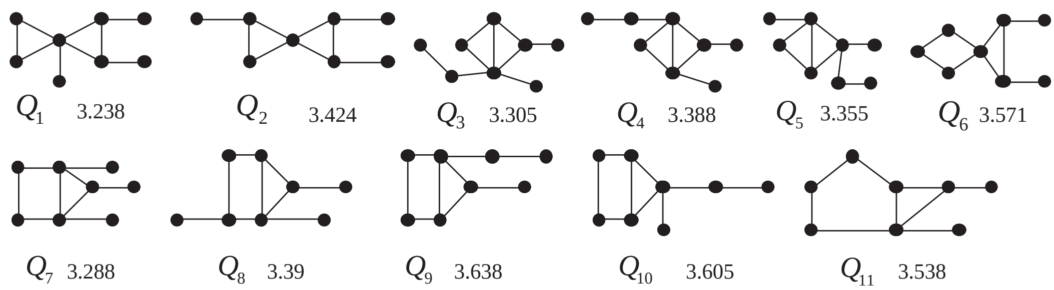

Figure 6

Subcase 2.2. There is no vertex of degree two on the two cycles of G, it means that the vertex u is on the path which join the two cycles.

In this subcase, there exists an edge vw which belongs to one of the two cycles of G such that $d(v) = 3, d(w) = 3$. Denote the other two vertices adjacent to v are v_1, v_2, the other two vertices adjacent to w are w_1, w_2. Without loss of generality, we have $d(v_1) = 1$, $3 \leq d(v_2) \leq 4$, $d(w_1) = 1$, $3 \leq d(w_2) \leq 4$. Let $G' = G - vw$.

Obviously, we have $G^{'} \in \mathscr{U}_{2m,m}(m \geq 6)$. By Theorem 3.1, we have

$$\begin{aligned} H(G) - \psi(2m,m) &= H(G^{'}) - \frac{2}{(2+d(v_2))(3+d(v_2))} - \frac{2}{(2+d(w_2))(3+d(w_2))} - \psi(2m,m) \\ &\geq \frac{1}{6} - \frac{8}{m+3} + \frac{2}{m+2} + \frac{6}{m+4} - \frac{2}{5\times 6} - \frac{2}{5\times 6} \\ &= \frac{2}{m+2} - \frac{2}{m+3} - \frac{6}{m+3} + \frac{6}{m+4} + \frac{1}{30} \\ &> \frac{m^2+7m+7}{30(m+3)(m+4)} > 0. \end{aligned}$$

Note that $H(R_8) = 3.193 < \psi(8,4) = 3.202$. Completing the proof. $\square$

Theorem 3.4. *Let $G \in \mathscr{B}_{n,m}(n \geq 2m, m \geq 5)$. Then $H(G) \geq \psi(n,m)$, with equality holds if and only if $G \cong B_{n,m}$.*

Proof. We apply induction on n. Suppose $n = 2m$. Then the theorem holds by Theorem 3.3. Now we suppose that $n > 2m$ and the result holds for smaller values of n.

If G has no pendant vertex, then clearly G is one of the type of $\{B_{2m+1}, B'_{2m+1}, Y_{2m+1}, Y'_{2m+1}, Y''_{2m+1}\}$ because G has an m-matching. It is easy to prove that $\min\{H(B_{2m+1}), H(B'_{2m+1}), H(Y_{2m+1}), H(Y'_{2m+1}), H(Y''_{2m+1})\} = H(Y_{2m+1}) = m + \frac{1}{3} > \psi(2m+1,m)$. So in the following proof, we assume that G has at least one pendant vertex.

By Lemma 2.3, G has an m-matching M and a pendant vertex v such that M does not saturate v. Let $uv \in E(G)$ with $d(u) = t$. Denote $N(u) \cap PV = \{v, x_1, \ldots, x_r\}$ and $N(u)\backslash PV = \{y_1, \ldots, y_{t-r-1}\}$. Then all $d(y_i) \geq 2$ $(1 \leq i \leq t-r-1)$. Let $G^{'} = G - v$. Then $G^{'} \in \mathscr{B}_{n-1,m}$. We have

$$\begin{aligned} H(G) &= H(G^{'}) + \frac{2r+2}{t+1} - \frac{2r}{t} + \sum_{i=1}^{t-r-1} \frac{2}{t+d(y_i)} - \sum_{i=1}^{t-r-1} \frac{2}{t+d(y_i)-1} \\ &\geq \psi(n-1,m) + \frac{2r+2}{t+1} + \frac{2(t-r-1)}{t+2} - \frac{2r}{t} - \frac{2(t-r-1)}{t+1} \\ &= \psi(n,m) + \frac{2(n-2m)}{n-m+2} + \frac{2m+2}{n-m+3} - \frac{2(n-2m+1)}{n-m+3} - \frac{2m+2}{n-m+4} \\ &\quad + \frac{2r+2}{t+1} + \frac{2(t-r-1)}{t+2} - \frac{2r}{t} - \frac{2(t-r-1)}{t+1} \\ &= \psi(n,m) + [\kappa(n-2m-1, n-m+1) - \kappa(n-2m, n-m+2)] - [\kappa(r-1,t-1) - \kappa(r,t)], \end{aligned}$$

where $\kappa(x,y)$ is defined in Lemma 2.4. Since the bicyclic graph G has an m-matching, $n - m + 2 \geq t$ and $n - 2m \geq r$. By Lemma 2.4 and $t \geq r+1$, we have

$$H(G) \geq \psi(n,m) + [\kappa(r-1, n-m+1) - \kappa(r, n-m+2)] - [\kappa(r-1,t-1) - \kappa(r,t)] \geq \psi(n,m).$$

The equality $H(G) = \psi(n,m)$ holds if and only if equality holds throughout the above inequalities, that is if and only if $G^{'} \cong B_{n-1,m}$, $d(y_1) = \ldots = d(y_{t-r-1}) = 2$, $n - m + 2 = t$ and $n - 2m = r$. Thus $G \cong B_{n,m}$. $\square$

Note 1. If $G \in \mathscr{B}_{2m,m}$, by Theorem 3.2, then $H(G) \leq m - \frac{1}{15}$ with equality if and only if $G \cong B_{2m}$ *or* B'_{2m}. Similarly, if $G \in \mathscr{B}_{2m+1,m}$, then $H(G) \leq m + \frac{13}{30}$ with equality if and only if $G \cong B_{2m+1}$ *or* B'_{2m+1}. As to $G \in \mathscr{B}_{n,m}$ $(n \geq 2m+2)$, we do not know the sharp upper bound on the harmonic index of bicyclic conjugated molecular graphs, this case maybe much more complicated.

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