MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **61** (2009) 419-442

ISSN 0340 - 6253

BIPARTITE BICYCLIC GRAPHS WITH LARGE ENERGIES

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(Received May 14, 2008)

Abstract

The energy of a graph is defined as the sum of the absolute values of its eigenvalues. Let $\mathcal{B}(n)$ be the class of bipartite bicyclic graphs on $n \geq 6$ vertices containing at least one pendent vertex. We determine the graphs with maximal energies in the class of graphs in $\mathcal{B}(n)$ of exactly three cycles, in the class of graphs in $\mathcal{B}(n)$ of exactly two cycles with a common vertex, and in the class of graphs in $\mathcal{B}(n)$ of two vertex-disjoint cycles, respectively.

1. INTRODUCTION

Let G be a simple graph on n vertices and $A(G)$ its adjacency matrix. The characteristic polynomial of G is the characteristic polynomial of $A(G)$, denoted by $\phi(G, \lambda)$. The roots of the equation $\phi(G, \lambda) = 0$, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, are called the eigenvalues of G [1]. The energy of G is defined as [2]

$$E(G) = \sum_{i=1}^{n} |\lambda_i|.$$

In theoretical chemistry, the energy of a graph has been extensively studied since it can be used to approximate the total π-electron energy of the molecule [2–5].

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Let G be a bipartite graph (depicting an alternant structure) on n vertices. Then [1, 3]

$$\phi(G,\lambda) = \sum_{i=0}^{\lfloor n/2 \rfloor} (-1)^i b_{2i}(G) \lambda^{n-2i},$$

where $b_{2i}(G) \geq 0$ for all $0 \leq i \leq \lfloor n/2 \rfloor$. A graph whose components are cycles and/or complete graphs with two vertices is called a Sachs graph. Sachs theorem [1, 3] states that for $1 \leq i \leq \lfloor n/2 \rfloor$,

$$b_{2i}(G) = (-1)^i \sum_{S \in L_{2i}} (-1)^{p(S)} 2^{c(S)},$$

where L_{2i} denotes the set of Sachs graphs of G with $2i$ vertices, $p(S)$ denotes the number of components of S and $c(S)$ denotes the number of cycles contained in S. In addition, $b_0(G) = 1$. Obviously, $b_2(G)$ equals the number of edges of G. For convenience, let $b_{2i}(G) = 0$ if $i < 0$ or $i > \lfloor n/2 \rfloor$. It is known that $E(G)$ can be expressed as the Coulson integral formula (see [3])

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \log \left[\sum_{i=0}^{\lfloor n/2 \rfloor} b_{2i}(G) x^{2i} \right] dx. \tag{1}$$

A quasi-order relation can be introduced in the class of all bipartite graphs: Let G_1 and G_2 be two bipartite graphs. If $b_{2i}(G_1) \leq b_{2i}(G_2)$ for all $i \geq 1$, then we write $G_1 \preceq G_2$. If $G_1 \preceq G_2$ and there exists a k such that $b_k(G_1) < b_k(G_2)$, then we write $G_1 \prec G_2$. From (1), we have the following increasing property on energy:

$$G_1 \prec G_2 \Rightarrow E(G_1) < E(G_2). \tag{2}$$

Thus, the coefficients in $\phi(G,\lambda)$ can be used to establish an ordering of bipartite graphs according to their energies.

A connected graph with n vertices and n edges is called a unicyclic graph, and a connected graph with n vertices and $n+1$ edges is called a bicyclic graph.

Gutman [6] determined the trees with minimal, second–minimal, third–minimal, and fourth–minimal energies, as well as the trees with maximal and second–maximal energies. Since then, graphs with minimal or maximal energies for many classes of graphs have been determined. For minimal energies, see [7–23]. Zhang *et al.* [24] determined hexagonal chains with maximal energy. Hou *et al.* [25] determined the bipartite unicyclic graphs with maximal energy. On the basis of the work in [26], Gutman *et al.* [27] determined the bipartite unicyclic graphs with second–maximal and third–maximal energies. Li and Zhang [28] showed that the graph obtained by attaching hexagons to the end vertices of a path on $n - 12$ vertices has the maximal energy among all n-vertex bipartite bicyclic graphs on $n \geq 16$ with the exception of the graphs obtained by connecting two vertex-disjoint cycles whose lengths are at least 10 and congruent 2 modulo 4 by an edge. By appropriate computer-based investigations, Furtula *et al.* [29] showed that this result holds for all n-vertex bipartite bicyclic graphs with $n > 12$. Related work on trees with third–maximal and fourth–maximal energies may be found in [30, 31].

Let $\mathcal{B}(n)$ be the class of bipartite bicyclic graphs on n vertices containing at least one pendent vertex (i.e., vertex of degree 1). Denote by $\mathcal{B}_1(n)$, $\mathcal{B}_2(n)$ and $\mathcal{B}_3(n)$ respectively the class of graphs in $\mathcal{B}(n)$ with exactly three cycles, the class of graphs in $\mathcal{B}(n)$ with exactly two cycles of a common vertex, and the class of graphs in $\mathcal{B}(n)$ with two vertex-disjoint cycles.

Note that the extremal graph in [28, 29] has no pendent vertices. In this paper, we study maximal energies of bicyclic graphs with at least one pendent vertex. We show that in the three classes $\mathcal{B}_1(n)$ $(n \geq 9)$, $\mathcal{B}_2(n)$ $(n \geq 12)$ and $\mathcal{B}_3(n)$ $(n \geq 15)$, the graphs B_n^1, B_n^2 and B_n^3 are the unique graphs with maximal energies, respectively, where the graphs B_n^1, B_n^2 and B_n^3 are shown in Fig. 1. Obviously, B_8^1, B_{11}^2 and B_{13}^3 are bipartite bicyclic graphs with no pendent vertices, and that B_n^1 $(n \geq 9)$, B_n^2 $(n \geq 12)$ and B_n^3 $(n \geq 14)$ have exactly one pendent vertex.

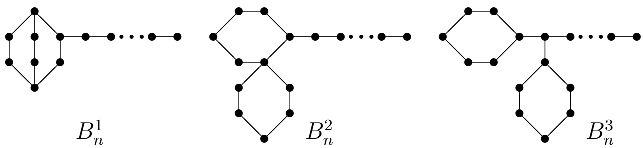


Figure 1: Graphs with maximal energies in $\mathcal{B}_1(n)$ $(n \geq 9)$, $\mathcal{B}_2(n)$ $(n \geq 12)$ and $\mathcal{B}_3(n)$ $(n \geq 15)$.

2. PRELIMINARIES

For two graphs G and H, $G \neq H$ means G and H are not isomorphic. For $v \in V(G)$, $\Gamma_G(v)$ denotes the set of neighbors of v in G and the degree of v is $\deg_G(v) = |\Gamma_G(v)|$. Denote by $V_p(G)$ the set of pendent vertices in G. Let $|G| = |V(G)|$. Let P_n and C_n be respectively the path and cycle on n vertices.

The maximum subgraph with no pendent vertices of a graph G is called the base graph of G, denoted by $\widehat{G}$. If $v \in V(\widehat{G})$ and $\deg_G(v) > \deg_{\widehat{G}}(v)$, then v is called a branching vertex of G.

For a graph G, denote by $d_G(u,v)$ the distance (length of a shortest path) between vertices u and v in G. For a vertex u and a subgraph H in G, let $d_G(u,H) = \min\{d_G(u,v)|v \in V(H)\}$. Obviously, if $u \in V(H)$ then $d_G(u,H) = 0$.

Let $\mathcal{C}(uv)$ be the set of cycles containing edge uv in G. Then [1, 3] $\phi(G,\lambda) = \phi(G-uv,\lambda) - \phi(G-u-v,\lambda) - 2\sum_{C\in\mathcal{C}(uv)} \phi(G-C,\lambda)$, from which the following lemma follows easily.

Lemma 2.1. *Let G be a bipartite graph.*

(i) If uv is a bridge in G, then

$$b_{2i}(G) = b_{2i}(G-uv) + b_{2i-2}(G-u-v),$$

in particular, if u is a pendent vertex, adjacent to v, then

$$b_{2i}(G) = b_{2i}(G-u) + b_{2i-2}(G-u-v).$$

(ii) If uv is an edge on some cycle, then

$$b_{2i}(G) = b_{2i}(G-uv) + b_{2i-2}(G-u-v) - 2\sum_{C_l\in\mathcal{C}(uv)} (-1)^{\frac{l}{2}} b_{2i-l}(G-C_l).$$

¿From Lemma 2.1 (i), we have

Lemma 2.2. *Let G be a bipartite graph. If H is obtained from G by deleting some bridges and/or pendent vertices, then $H \preceq G$.*

For $1 \le t < n$, let $P_{n,k,t}$ be the tree obtained by attaching a path P_t to vertex v_k of the path P_{n-t} labeled consecutively by $v_1, v_2, \ldots, v_{n-t}$. Let P_n^l be the unicyclic graph obtained by attaching a path P_{n-l} to a vertex of the cycle C_l for $l < n$. Let $P^l_{n,k,t}$ be the unicyclic graph obtained by identifying a vertex of a cycle C_l and vertex $v_{n-l-t+1}$ of the tree $P_{n-l+1,k,t}$. For convenience, let $Q_n = P_{n,3,2} = P_{n,3,n-5}$ for $n \geq 6$ and $P^l_l = C_l$. Let $B^*_{n,a,b}$ be the graph obtained by connecting a vertex in C_a and a vertex in C_b by a path when $n \geq a+b$ and the graph consisting of two cycles C_a and C_b with a common vertex when $n = a+b-1$. For convenience, let $B^*_n = B^*_{n,6,6}$.

Lemma 2.3. [3] *Let T be an acyclic graph on $n \geq 6$ vertices and $T \neq P_n, Q_n$. Then $T \prec Q_n \prec P_n$.*

Lemma 2.4. [25] *Let G be a bipartite graph on n vertices containing a unique cycle of length l with $l \equiv 2 \pmod 4$. Then $G \preceq P^l_n$.*

Lemma 2.5. [25] *Let G be a bipartite graph on n vertices containing a unique cycle and $G \neq C_n$. Then $G \preceq P^6_n$.*

Lemma 2.6. [3] *Let $n = 4k, 4k+1, 4k+2$ or $4k+3$. Then*

$$\begin{aligned} P_1 \cup P_{n-1} \preceq & P_3 \cup P_{n-3} \preceq \cdots \preceq P_{2k-1} \cup P_{n-2k+1} \preceq P_{2k+1} \cup P_{n-2k-1} \\ & \preceq P_{2k} \cup P_{n-2k} \preceq \cdots \preceq P_4 \cup P_{n-4} \preceq P_2 \cup P_{n-2}. \end{aligned}$$

Lemma 2.7. *(i) For $n \geq 11$, $1 \leq t \leq n-7$ and $t \neq 2, n-8$, $P_t \cup P^6_{n-t} \preceq P_4 \cup P^6_{n-4}$.*

(ii) For $n \geq 8$ and $1 \leq t \leq n-7$, $P_t \cup P^6_{n-t} \prec P_{n-6} \cup C_6$.

(iii) For $n \geq 8$, $P_n \prec P_{n-6} \cup C_6$.

Proof. ¿From Lemma 2.1 (ii),

$$b_{2i}(P_s \cup P^6_{n-s}) = b_{2i}(P_s \cup P_{n-s}) + b_{2i-2}(P_4 \cup P_s \cup P_{n-s-6}) + 2b_{2i-6}(P_s \cup P_{n-s-6}),$$

where $1 \leq s \leq n-7$. By Lemma 2.6, $P_t \cup P_{n-t} \preceq P_4 \cup P_{n-4}$ and $P_t \cup P_{n-t-6} \preceq P_4 \cup P_{n-10}$. Thus $P_t \cup P^6_{n-t} \preceq P_4 \cup P^6_{n-4}$. This proves (i)

The result in (ii) is true for $n = 8$ by Sachs theorem. For $n \geq 9$, since $P_t \cup P^6_{n-t} \preceq P_2 \cup P^6_{n-2}$, by similar arguments as above, we need only to show that $P_2 \cup P^6_{n-2} \prec P_{n-6} \cup C_6$. By Lemma 2.1 (i),

$$\begin{aligned} b_{2i}(P_2 \cup P^6_{n-2}) &= b_{2i}(P_2 \cup P_{n-8} \cup C_6) + b_{2i-2}(P_2 \cup P_5 \cup P_{n-9}), \\ b_{2i}(P_{n-6} \cup C_6) &= b_{2i}(P_2 \cup P_{n-8} \cup C_6) + b_{2i-2}(P_1 \cup P_{n-9} \cup C_6). \end{aligned}$$

By Sachs theorem, $P_2 \cup P_5 \prec P_1 \cup C_6$. Thus $P_2 \cup P_{n-2}^6 \prec P_{n-6} \cup C_6$. This proves (ii).

The result in (iii) is true for $n = 8, 9$ by Sachs theorem. For $n \geq 10$, by Lemmas 2.1 and 2.6,

$$\begin{aligned} b_{2i}(P_n) &= b_{2i}(P_6 \cup P_{n-6}) + b_{2i-2}(P_5 \cup P_{n-7}) \\ &\leq b_{2i}(P_6 \cup P_{n-6}) + b_{2i-2}(P_4 \cup P_{n-6}) \\ &= b_{2i}(P_{n-6} \cup C_6) - 2b_{2i-6}(P_{n-6}). \end{aligned}$$

Thus $b_{2i}(P_n) \leq b_{2i}(P_{n-6} \cup C_6)$ and $b_6(P_n) < b_6(P_{n-6} \cup C_6)$, implying $P_n \prec P_{n-6} \cup C_6$. This proves (iii). □

By Lemmas 2.1 (ii) and 2.7 (ii), we have

Lemma 2.8. *For* $6 \leq t \leq n - 6$, $P_t^6 \cup P_{n-t}^6 \preceq P_{n-6}^6 \cup C_6$.

By Lemma 2.1 (i), we have

Lemma 2.9. *Let* G, G' *be two bipartite graphs and* u *(resp.* u'*) a pendent vertex, adjacent to* v *(resp.* v'*), of the graph* G *(resp.* G'*). If* $G - u \preceq G' - u'$ *and* $G - u - v \prec G' - u' - v'$*, or* $G - u \prec G' - u'$ *and* $G - u - v \preceq G' - u' - v'$*, then* $G \prec G'$.

3. GRAPHS IN $\mathcal{B}_1(n)$ WITH MAXIMAL ENERGY

By Lemma 2.1 (ii), it is easily seen that $P_n \prec P_n^6$ for $n \geq 6$ and $P_n^6 \prec B_n^1$ for $n \geq 8$.

Lemma 3.1. *Let* $G \in \mathcal{B}_1(n)$*, where* $|\widehat{G}| < 8$ *and* $n \geq 8$*. Then* $G \prec B_n^1$.

Proof. We prove the lemma by induction on n.

Suppose that $n = 8$. Take a vertex $z \in V(\widehat{G})$ with $\deg_{\widehat{G}}(z) = 3$ and $w \in \Gamma_{\widehat{G}}(z)$ such that $G - z - w \neq P_6$. Obviously, zw lies on two cycles, say C_b and C_c with $b \leq c$. By Lemmas 2.1 (ii), 2.3 and 2.5,

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G - zw) + b_{2i-2}(G - z - w) - 2\textstyle\sum_{l \in \{b,c\}} (-1)^{\frac{l}{2}} b_{2i-l}(G - C_l) \\ &\leq b_{2i}(P_8^6) + b_{2i-2}(Q_6) + 4b_{2i-6}(P_2) = b_{2i}(B_8^1), \end{aligned}$$

implying $G \preceq B_8^1$. Since $b_2(G - C_b) < b_2(P_2)$ if $b = 6$ or $-b_2(G - C_b) < b_2(P_2)$ if $b = 4$, we have $b_8(G) < b_8(B_8^1)$. Thus $G \prec B_8^1$.

Suppose that $n = 9$. Suppose that $d_G(u, \widehat{G}) = 1$ for some $u \in V_p(G)$. Then $G - u \in \mathcal{B}_1(8)$ and so $G - u \prec B_8^1$. Let $v \in \Gamma_G(u)$. If $G - u - v$ is an acyclic graph, then by Lemma 2.3, $G - u - v \preceq P_7 \prec P_7^6$. Otherwise, $G - u - v$ contains a unique cycle, and then by Lemma 2.5, $G - u - v \preceq P_7^6$. Thus, by Lemma 2.9, $G \prec B_9^1$.

Suppose that $d_G(u, \widehat{G}) \geq 2$ for any $u \in V_p(G)$. Obviously, G has at most two branching vertices. If $\widehat{G} = A_6$ or A_7, where A_6, A_7 are the bicyclic graphs obtained respectively by identifying an edge of two quadrangles and by identifying two adjacent edges of a quadrangle and a hexagon, then by Sachs theorem, $G \prec B_9^1$. Otherwise, $\widehat{G}$ is the complete bipartite graph $K_{2,3}$ with bipartition $(\{v_1, v_2\}, \{v_3, v_4, v_5\})$, and one of v_3, v_4, v_5, say v_3, is not a branching vertex of G. Then by Lemmas 2.1, 2.2, 2.3, 2.5 and 2.6,

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G - v_1v_3 - v_3v_2) + b_{2i-2}(G - v_3 - v_2 - v_4v_1) \\ &\quad + b_{2i-2}(G - v_1 - v_3 - v_2v_4) - 2b_{2i-4}(G - v_1 - v_3 - v_2 - v_5) \\ &\leq b_{2i}(P_8^6) + b_{2i-2}(P_2 \cup P_5) + b_{2i-2}(P_2 \cup P_5) \\ &\leq b_{2i}(P_8^6) + b_{2i-2}(P_1 \cup C_6) + b_{2i-2}(Q_7) = b_{2i}(B_9^1) - 4b_{2i-6}(P_2). \end{aligned}$$

Thus $b_{2i}(G) \leq b_{2i}(B_9^1)$ and $b_6(G) < b_6(B_9^1)$, implying $G \prec B_9^1$.

Now suppose that $n \geq 10$, the result holds for $n-1$ and $n-2$. Let $G \in \mathcal{B}_1(n)$. Let $u \in V_p(G)$ such that $d_G(u, \widehat{G}) = \max\{d_G(x, \widehat{G}) | x \in V_p(G)\}$ and let v be the unique neighbor of u. Obviously, $G - u \in \mathcal{B}_1(n-1)$ and thus by the induction hypothesis, $G - u \prec B_{n-1}^1$.

Case 1. $d_G(u, \widehat{G}) = 1$. If $G - u - v$ is an acyclic graph, then by Lemma 2.3, $G - u - v \preceq P_{n-2} \prec B_{n-2}^1$. Otherwise, $G - u - v$ contains a unique cycle, and then by Lemma 2.5, $G - u - v \preceq P_{n-2}^6 \prec B_{n-2}^1$.

Case 2. $d_G(u, \widehat{G}) \geq 2$. If $G - u - v$ is disconnected, then $G - u - v$ is a subgraph of G', where $G' \in \mathcal{B}_1(n-2)$ is obtained from $G - u - v$ by attaching all isolated vertices of $G - u - v$ to a vertex of $\widehat{G}$, and by the induction hypothesis and Lemma 2.2, $G - u - v \prec G' \prec B_{n-2}^1$. If $G - u - v$ is connected, then $G - u - v \in \mathcal{B}_1(n-2)$, and by the induction hypothesis, $G - u - v \prec B_{n-2}^1$.

Combining Cases 1 and 2, $G - u - v \prec B_{n-2}^1$. Now by Lemma 2.9, $G \prec B_n^1$. $\square$

Lemma 3.2. *Let $G \in \mathcal{B}_1(n)$, where $n = |\widehat{G}| + 2$, $|\widehat{G}| \geq 8$, $|V_p(G)| = 1$ and $G \neq B_n^1$. Then $G \prec B_n^1$.*

Proof. Let x be the unique pendent vertex of G. Let u be the neighbor of x and v the unique branching vertex of G. Obviously, $n \geq 10$.

Case 1. $\deg_G(v) = 4$. If G is the bicyclic graph obtained by attaching a path P_2 to a vertex of degree 3 in B_8^1, then $n = 10$ and it can be checked by Sachs theorem that $G \prec B_{10}^1$. Otherwise, we take $w \in \Gamma_{\widehat{G}}(v)$ such that vw lies on two cycles C_b and C_c with $c \neq 6$. By Lemmas 2.1, 2.3 and 2.5,

$$\begin{aligned}
b_{2i}(G) &= b_{2i}(G - vw) + b_{2i-2}(G - v - w) - 2\textstyle\sum_{l \in \{b,c\}} (-1)^{\frac{l}{2}} b_{2i-l}(G - C_l) \\
&\leq b_{2i}(P_n^6) + b_{2i-2}(P_2 \cup P_{n-4}) - 2\textstyle\sum_{l \in \{b,c\}} (-1)^{\frac{l}{2}} b_{2i-l}(P_2 \cup P_{n-l-2}) \\
&= b_{2i}(P_n^6) + b_{2i-2}(P_2 \cup P_4 \cup P_{n-8}) + b_{2i-4}(P_2 \cup P_{n-9}) \\
&\quad +2b_{2i-6}(P_2 \cup P_{n-9}) - 2\textstyle\sum_{l \in \{b,c\}} (-1)^{\frac{l}{2}} b_{2i-l}(P_2 \cup P_{n-l-2}), \\
b_{2i}(B_n^1) &= b_{2i}(P_n^6) + b_{2i-2}(Q_6 \cup P_{n-8}) + 4b_{2i-6}(P_2 \cup P_{n-8}) \\
&= b_{2i}(P_n^6) + b_{2i-2}(P_2 \cup P_4 \cup P_{n-8}) + b_{2i-4}(P_2 \cup P_{n-8}) \\
&\quad +2b_{2i-6}(P_2 \cup P_{n-9}) + 2b_{2i-6}(P_2 \cup P_{n-8}) + 2b_{2i-8}(P_2 \cup P_{n-10}).
\end{aligned}$$

By Lemma 2.2, $b_{2i-4}(P_2 \cup P_{n-9}) \leq b_{2i-4}(P_2 \cup P_{n-8})$, and by Lemma 2.1 (i), $2b_{2i-c}(P_2 \cup P_{n-c-2}) \leq \cdots \leq 2b_{2i-10}(P_2 \cup P_{n-12}) \leq 2b_{2i-8}(P_2 \cup P_{n-10})$ if $c \equiv 2 \pmod 4$ or $-2b_{2i-c}(P_2 \cup P_{n-c-2}) \leq 2b_{2i-8}(P_2 \cup P_{n-10})$ if $c \equiv 0 \pmod 4$. Note that $-(-1)^{\frac{b}{2}} 2b_{2i-b}(P_2 \cup P_{n-b-2}) \leq 2b_{2i-6}(P_2 \cup P_{n-8})$. Then $b_{2i}(G) \leq b_{2i}(B_n^1)$. Since $b_2(P_2 \cup P_{n-9}) < b_2(P_2 \cup P_{n-8})$, we have $b_6(G) < b_6(B_n^1)$. Thus $G \prec B_n^1$.

Case 2. $\deg_G(v) = 3$. Obviously, v lies outside some cycle, say C_a. Take a vertex $w \in V(\widehat{G})$ such that $d_{\widehat{G}}(w, C_a) = 1$. Let z be the neighbor of w in C_a. Then zw lies on the other two cycles, say C_b and C_c. Let G' be the graph obtained from G by removing edge uv and adding edge uw.

If $a \equiv 2 \pmod 4$, then either $b \neq 6$ or $c \neq 6$ and by similar arguments as those in Case 1, $G' \prec B_n^1$. So, to prove $G \prec B_n^1$, it suffices to prove $G \preceq G'$. By Lemmas 2.1 (i) and 2.4, $b_{2i}(G) \leq b_{2i}(P_2 \cup \widehat{G}) + b_{2i-2}(P_1 \cup P_{n-3}^a) = b_{2i}(G')$, implying $G \preceq G'$.

Suppose that $a \equiv 0 \pmod 4$. Suppose that $d_{\widehat{G}}(v, C_a) = 1$. Then $G = G'$. If $b \neq 6$ or $c \neq 6$, then by similar arguments as those in Case 1, $G \prec B_n^1$. If $b = c = 6$, then G must be the bicyclic graph obtained from P_{11}^8 by adding edge wy between the neighbor of z outside the cycle C_8 and the vertex (in the cycle) of distance 4 from z, where z is the unique vertex of degree 3 in P_{11}^8, and by Sachs theorem, $G \prec B_{11}^1$. Now suppose that $d_{\widehat{G}}(v, C_a) \geq 2$. Then we can take two vertices w and z as above such that $G - z - w \neq P_{n-2}$. By Lemmas 2.1 (ii) and 2.3,

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G - zw) + b_{2i-2}(G - z - w) - 2\sum_{l\in\{b,c\}} (-1)^{\frac{l}{2}} b_{2i-l}(G - C_l) \\ &\leq b_{2i}(P_{n,k,2}^a) + b_{2i-2}(Q_{n-2}) - 2\sum_{l\in\{b,c\}} (-1)^{\frac{l}{2}} b_{2i-l}(P_2 \cup P_{n-l-2}), \\ b_{2i}(B_n^1) &= b_{2i}(P_{n,n-7,1}^6) + b_{2i-2}(Q_{n-2}) + 4b_{2i-6}(P_2 \cup P_{n-8}), \end{aligned}$$

where $1 < k < n-a-2$. So to prove $G \prec B_n^1$, we need only to prove $P_{n,k,2}^a \prec P_{n,n-7,1}^6$.

If $a = 4$, then by Lemma 2.1,

$$b_{2i}(P_{n,k,2}^4) = b_{2i}(P_{n-1,k,2}) + b_{2i-2}(P_{n-3,k,2}) + b_{2i-2}(P_{n-4,k,2}),$$

$$b_{2i}(P_{n,n-7,1}^6) = b_{2i}(P_{n-1}) + b_{2i-2}(P_6 \cup P_{n-8}) + b_{2i-2}(P_4 \cup P_{n-6}) + 2b_{2i-6}(P_{n-6}).$$

By Lemma 2.3, $b_{2i}(P_{n-1,k,2}) \leq b_{2i}(P_{n-1})$, and by Lemma 2.6, $b_{2i-2}(P_{n-3,k,2}) \leq b_{2i-2}(P_6 \cup P_{n-8})$. Note that $b_{2i-2}(P_{n-4,k,2}) \leq b_{2i-2}(P_4 \cup P_{n-6})$ and that $b_6(P_{n,k,2}^4) < b_6(P_{n,n-7,1}^6)$. We have $P_{n,k,2}^4 \prec P_{n,n-7,1}^6$.

If $a \geq 8$, then by Lemmas 2.1 and 2.3,

$$\begin{aligned} b_{2i}(P_{n,k,2}^a) &= b_{2i}(P_{n,k,2}) + b_{2i-2}(P_{a-2} \cup P_{n-a,k,2}) - 2b_{2i-a}(P_{n-a,k,2}) \\ &= b_{2i}(P_{n-2}) + b_{2i-2}(P_{n-2}) + b_{2i-2}(P_{k-1} \cup P_{n-k-2}) \\ &\quad + b_{2i-2}(P_{a-2} \cup P_{n-a,k,2}) - 2b_{2i-a}(P_{n-a,k,2}) \\ &\leq b_{2i}(P_{n-2}) + b_{2i-2}(P_6 \cup P_{n-8}) + b_{2i-2}(P_{k-1} \cup P_{n-k-2}) \\ &\quad + b_{2i-2}(P_{a-2} \cup P_{n-a}) + b_{2i-4}(P_3 \cup P_{n-9}) \\ &\quad + b_{2i-6}(P_2 \cup P_{n-9}) + b_{2i-6}(P_3 \cup P_{n-9}), \\ b_{2i}(P_{n,n-7,1}^6) &= b_{2i}(P_{n-2}) + b_{2i-2}(P_6 \cup P_{n-8}) + b_{2i-2}(P_{k-1} \cup P_{n-k-2}) \\ &\quad + b_{2i-2}(P_4 \cup P_{n-6}) + b_{2i-4}(P_{k-2} \cup P_{n-k-3}) + 2b_{2i-6}(P_{n-6}). \end{aligned}$$

By Lemma 2.6, $b_{2i-2}(P_{a-2} \cup P_{n-a}) \leq b_{2i-2}(P_4 \cup P_{n-6})$, and by Lemma 2.2, $b_{2i-6}(P_2 \cup P_{n-9}) + b_{2i-6}(P_3 \cup P_{n-9}) \leq 2b_{2i-6}(P_{n-6})$. Note that $b_{2i-4}(P_3 \cup P_{n-9}) \leq b_{2i-4}(P_{k-2} \cup P_{n-k-3})$ and that $b_2(P_2 \cup P_{n-9}) < b_2(P_{n-6})$. We have $P_{n,k,2}^a \prec P_{n,n-7,1}^6$. $\square$

Similarly, we have

Lemma 3.3. *Let $G \in \mathcal{B}_1(n)$, where $n = |\widehat{G}|+1$, $|\widehat{G}| \geq 8$ and $G \neq B_n^1$. Then $G \prec B_n^1$.*

Lemma 3.4. *Let $G \in \mathcal{B}_1(n)$, where $|\widehat{G}| \geq 8$, $G \neq B_n^1$ and $n \geq 9$. Then $G \prec B_n^1$.*

Proof. We prove the lemma by induction on $n - |\widehat{G}|$.

By Lemma 3.3, the result is true for $n - |\widehat{G}| = 1$. Let $h \geq 2$ and suppose that the result holds for $1 \leq n - |\widehat{G}| < h$. Let $G \in \mathcal{B}_1(n)$ and $n - |\widehat{G}| = h$.

Let $u \in V_p(G)$ such that $d_G(u, \widehat{G}) = \max\{d_G(x, \widehat{G}) | x \in V_p(G)\}$ and let v be the unique neighbor of u. Obviously, $G - u \in \mathcal{B}_1(n-1)$ and thus by the induction hypothesis, $G - u \prec B_{n-1}^1$ if $G - u \neq B_{n-1}^1$.

Case 1. $d_G(u, \widehat{G}) = 1$. If $G - u - v$ is an acyclic graph, and by Lemma 2.3, $G - u - v \preceq P_{n-2} \prec B_{n-2}^1$. Otherwise, $G - u - v$ contains a unique cycle, and then by Lemma 2.5, $G - u - v \preceq P_{n-2}^6 \prec B_{n-2}^1$. So, by Lemma 2.9, $G \prec B_n^1$.

Case 2. $d_G(u, \widehat{G}) \geq 2$. If $G - u - v$ is disconnected, then $G - u - v$ is a subgraph of G', where $G' \in \mathcal{B}_1(n-2)$ is obtained from $G - u - v$ by attaching all isolated vertices of $G - u - v$ to a vertex of $\widehat{G}$, and by the induction hypothesis and Lemma 2.2, $G - u - v \prec G' \preceq B_{n-2}^1$. Thus, by Lemma 2.9, $G \prec B_n^1$. Suppose that $G - u - v$ is connected. If $n - |\widehat{G}| = 2$, then by Lemma 3.2, $G \prec B_n^1$. If $n - |\widehat{G}| \geq 3$, then $G - u - v \in \mathcal{B}_1(n-2)$ and $G - u \neq B_{n-1}^1$, and thus by the induction hypothesis, $G - u - v \preceq B_{n-2}^1$. So, by Lemma 2.9, $G \prec B_n^1$. □

Combining Lemmas 3.1 and 3.4, and using the increasing property (2), we obtain the following theorem.

Theorem 3.1. *Let $G \in \mathcal{B}_1(n)$, where $G \neq B_n^1$ and $n \geq 9$. Then $G \prec B_n^1$ and $E(G) < E(B_n^1)$.*

Remark. Let $A_6^1, A_7^1, A_7^{1'}$ and A_8^1 be the graphs shown in Fig. 2. For $n = 6, 7, 8$, we have

(i) if $G \in \mathcal{B}_1(n)$ with $G \neq A_n^1$, then $G \prec A_n^1$ and $E(G) < E(A_n^1)$ for $n = 6, 8$,

(ii) if $G \in \mathcal{B}_1(7)$ with $G \neq A_7^1, A_7^{1'}$, then $G \prec A_7^1, A_7^{1'}$, and $E(G) < E(A_7^{1'}) = 8.5702 < E(A_7^1) = 8.6332$.

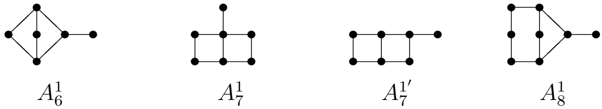


Figure 2: Graphs with maximal energies and a related graph in $\mathcal{B}_1(n)$, where $n = 6, 7, 8$.

4. GRAPHS IN $\mathcal{B}_2(n)$ WITH MAXIMAL ENERGY

By Lemma 2.1 (ii), it is easily seen that $P_n^6 \prec B_n^2$ for $n \geq 11$.

Lemma 4.1. *Let $G \in \mathcal{B}_2(n)$, where $|\widehat{G}| < 11$ and $n \geq 11$. Then $G \prec B_n^2$.*

Proof. We prove the lemma by induction on n.

Suppose that $n = 11$. Take the vertex $z \in V(\widehat{G})$ with $\deg_{\widehat{G}}(z) = 4$ and $w \in \Gamma_{\widehat{G}}(z)$ such that $G - zw \neq P_{11}^6$, $G - z - w \neq P_2 \cup P_7$. Obviously, zw lies on one cycle, say C_b. By Lemmas 2.1 (ii), 2.3, 2.5 and 2.6,

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G - zw) + b_{2i-2}(G - z - w) - (-1)^{\frac{b}{2}} 2b_{2i-b}(G - C_b) \\ &\leq b_{2i}(P_{11}^6) + b_{2i-2}(P_4 \cup P_5) + 2b_{2i-6}(P_5) = b_{2i}(B_{11}^2). \end{aligned}$$

Note that $G - zw \prec P_{11}^6$. We have $G \prec B_{11}^2$.

Suppose that $n = 12$. Suppose that $d_G(u, \widehat{G}) = 1$ for some $u \in V_p(G)$. Then $G - u \in \mathcal{B}_2(11)$ and thus $G - u \prec B_{11}^2$. Let $v \in \Gamma_G(u)$. If $G - u - v$ is an acyclic graph, then by Lemma 2.3, $G - u - v \preceq P_{10} \prec P_{10}^6$. If $G - u - v$ contains a cycle, then by Lemma 2.5, $G - u - v \preceq P_{10}^6$. Therefore, by Lemma 2.9, $G \prec B_{12}^2$.

Now suppose that $d_G(u, \widehat{G}) \geq 2$ for any $u \in V_p(G)$. Obviously, there is at most one branching vertex in a quadrangle of G, denoted by $v_1v_2v_3v_4v_1$. Suppose without loss of generality that $\deg_{\widehat{G}}(v_1) = 4$ and v_2 is not a branching vertex. By Lemmas 2.1, 2.3, 2.5 and 2.6,

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G - v_1v_2 - v_2v_3) + b_{2i-2}(G - v_2 - v_3 - v_4v_1) \\ &\quad + b_{2i-2}(G - v_1 - v_2 - v_3v_4) \\ &\leq b_{2i}(P_{11}^6) + b_{2i-2}(P_{10}^6) + b_{2i-2}(P_1 \cup P_4 \cup P_5) \\ &= b_{2i}(B_{12}^2) - 2b_{2i-6}(P_1 \cup P_5). \end{aligned}$$

Therefore $G \preceq B_{12}^2$ and $b_6(G) < b_6(B_{12}^2)$, implying $G \prec B_{12}^2$.

Suppose that $n \geq 13$, the result holds for $n-1$ and $n-2$, and $G \in \mathcal{B}_2(n)$. By similar arguments as those in Lemma 3.1, we have $G \prec B_n^2$. $\square$

Let $B_{n,b}^a$ be the graph obtained from $B_{a+b-1,a,b}^*$ by attaching a path $P_{n-a-b+1}$ to a vertex $w \in V(B_{a+b-1,a,b}^*)$ with $d_{B_{a+b-1,a,b}^*}(w, C_a) = 1$.

Lemma 4.2. *Let* $G \in \mathcal{B}_2(n)$*, where* $n = |\widehat{G}| + 2$*,* $|\widehat{G}| \geq 11$*,* $|V_p(G)| = 1$ *and* $G \neq B_n^2$*. Then* $G \prec B_n^2$*.*

Proof. Let x be the unique pendent vertex of G, and let u be the neighbor of x and v the unique branching vertex in G. Let C_a and C_b be the two cycles of G. Suppose that v lies on C_b. Then $n = a + b + 1$.

Claim 1. $G \preceq B_{n,b}^a$ for $G \neq B_{n,b}^a$.

By Lemma 2.1 (i),

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G - uv) + b_{2i-2}(G - u - v), \\ b_{2i}(B_{n,b}^a) &= b_{2i}(P_2 \cup B_{n-2,a,b}^*) + b_{2i-2}(P_1 \cup P_{n-3}^a). \end{aligned}$$

If $\deg_{\widehat{G}}(v) = 4$, then $G-u-v = P_1 \cup P_{a-1} \cup P_{b-1}$, and by Lemma 2.1, $b_{2i-2}(G-u-v) \leq b_{2i-2}(P_1 \cup P_{n-3}^a)$. If $\deg_{\widehat{G}}(v) = 2$, then $G-u-v = P_1 \cup P_{n-3,k,t}^a$, where $1 \leq t \leq n-a-4$ and $k = n - a - t - 2$, and by Lemma 2.1,

$$\begin{aligned} b_{2i-2}(G - u - v) &= b_{2i-2}(P_t \cup P_{n-t-3}^a) + b_{2i-4}(P_{t-1} \cup P_{a-1} \cup P_{n-a-t-3}) \\ &\leq b_{2i-2}(P_t \cup P_{n-t-3}^a) + b_{2i-4}(P_{t-1} \cup P_{n-t-4}^a) \\ &= b_{2i-2}(P_1 \cup P_{n-3}^a). \end{aligned}$$

Clearly, $b_{2i}(G - uv) = b_{2i}(P_2 \cup B_{n-2,a,b}^*)$. Hence $G \preceq B_{n,b}^a$.

Claim 2. If $B_{n,b}^a \neq B_n^2$, then $B_{n,b}^a \prec B_n^2$.

Case 1. $b = 4$. Then $n = a + 5$ and $a \geq 8$. By Lemma 2.1,

$$\begin{aligned} b_{2i}(B_{n,4}^a) &= b_{2i}(P_n^a) + b_{2i-2}(P_2 \cup P_2 \cup P_{a-1}) - 2b_{2i-4}(P_2 \cup P_{a-1}) \\ &= b_{2i}(P_n^a) + b_{2i-2}(P_2 \cup P_{a-1}) - b_{2i-4}(P_2 \cup P_{a-1}), \\ b_{2i}(B_n^2) &= b_{2i}(P_n^6) + b_{2i-2}(P_4 \cup P_5 \cup P_{a-6}) + 2b_{2i-6}(P_5 \cup P_{a-6}). \end{aligned}$$

By Lemma 2.5, $b_{2i}(P_n^a) \le b_{2i}(P_n^6)$, and by Lemmas 2.2 and 2.6, $b_{2i-2}(P_2 \cup P_{a-1}) \le b_{2i-2}(P_{a+1}) \le b_{2i-2}(P_4 \cup P_5 \cup P_{a-6})$. Thus $B_{n,4}^a \preceq B_n^2$ and $b_6(B_{n,4}^a) < b_6(B_n^2)$, implying $B_{n,4}^a \prec B_n^2$.

Case 2. $b \ge 6$. By Lemma 2.1,

$$\begin{aligned} b_{2i}(B_{n,b}^a) &= b_{2i}(P_n^a) + b_{2i-2}(P_2 \cup P_{b-2} \cup P_{a-1}) - (-1)^{\frac{b}{2}} 2b_{2i-b}(P_2 \cup P_{a-1}) \\ &= b_{2i}(P_n^a) + b_{2i-2}(P_2 \cup P_2 \cup P_{b-4} \cup P_{a-1}) + b_{2i-4}(P_{b-5} \cup P_{a-1}) \\ &\quad + b_{2i-6}(P_{b-5} \cup P_{a-1}) - (-1)^{\frac{b}{2}} 2b_{2i-b}(P_2 \cup P_{a-1}), \\ b_{2i}(B_{n,6}^a) &= b_{2i}(P_n^a) + b_{2i-2}(P_4 \cup P_{b-4} \cup P_{a-1}) + 2b_{2i-6}(P_{b-4} \cup P_{a-1}) \\ &= b_{2i}(P_n^a) + b_{2i-2}(P_2 \cup P_2 \cup P_{b-4} \cup P_{a-1}) + b_{2i-4}(P_{b-4} \cup P_{a-1}) \\ &\quad + 2b_{2i-6}(P_{b-5} \cup P_{a-1}) + 2b_{2i-8}(P_{b-6} \cup P_{a-1}). \end{aligned}$$

By Lemma 2.2, $b_{2i-4}(P_{b-5} \cup P_{a-1}) \le b_{2i-4}(P_{b-4} \cup P_{a-1})$. Thus $B_{n,b}^a \preceq B_{n,6}^a$ and $b_2(P_{b-5} \cup P_{a-1}) < b_2(P_{b-4} \cup P_{a-1})$, implying $B_{n,b}^a \prec B_{n,6}^a$ for $b \ge 8$.

By Lemma 2.1 (i),

$$\begin{aligned} b_{2i}(B_{n,6}^a) &= b_{2i}(P_{n-a-5} \cup B_{a+5,a,6}^*) + b_{2i-2}(P_{n-a-6} \cup P_{a+4}^a), \\ b_{2i}(B_{n,a}^6) &= b_{2i}(P_{n-a-5} \cup B_{a+5,a,6}^*) + b_{2i-2}(P_{n-a-6} \cup P_{a+4}^6). \end{aligned}$$

By Lemma 2.5, $b_{2i-2}(P_{n-a-6} \cup P_{a+4}^a) \le b_{2i-2}(P_{n-a-6} \cup P_{a+4}^6)$. Thus $B_{n,6}^a \preceq B_{n,a}^6$.

By Lemma 2.1 (ii),

$$b_{2i}(B_n^2) = b_{2i}(P_n^6) + b_{2i-2}(P_4 \cup P_5 \cup P_{n-11}) + 2b_{2i-6}(P_5 \cup P_{n-11}).$$

If $a = 4$, then by Lemma 2.1 (ii),

$$b_{2i}(B_{n,4}^6) = b_{2i}(P_n^6) + b_{2i-2}(P_1 \cup P_1 \cup P_5 \cup P_{n-9}) - b_{2i-4}(P_5 \cup P_{n-9}).$$

By Lemmas 2.2 and 2.6, $b_{2i-2}(P_1 \cup P_1 \cup P_5 \cup P_{n-9}) \le b_{2i-2}(P_4 \cup P_5 \cup P_{n-11})$. Thus $B_{n,4}^6 \preceq B_n^2$ and $b_6(B_{n,4}^6) < b_6(B_n^2)$, implying $B_{n,4}^6 \prec B_n^2$.

Suppose that $a \ge 8$. Then by Lemma 2.1 (ii),

$$b_{2i}(B_{n,a}^6) = b_{2i}(P_n^6) + b_{2i-2}(P_{a-2} \cup P_5 \cup P_{n-a-5}) - (-1)^{\frac{a}{2}} 2b_{2i-a}(P_5 \cup P_{n-a-5}).$$

If $n = a+7$, then $B_{n,a}^6 \prec B_n^2$ as above. If $n \ne a+7$, then by Lemma 2.6, $b_{2i-2}(P_{a-2} \cup P_5 \cup P_{n-a-5}) \le b_{2i-2}(P_4 \cup P_5 \cup P_{n-11})$. Thus $B_{n,a}^6 \preceq B_n^2$ and $b_6(B_{n,a}^6) < b_6(B_n^2)$, implying $B_{n,a}^6 \prec B_n^2$. □

Similarly, we have

Lemma 4.3. *Let* $G \in \mathcal{B}_2(n)$*, where* $n = |\widehat{G}| + 1$*,* $|\widehat{G}| \geq 11$ *and* $G \neq B_n^2$*. Then* $G \prec B_n^2$*.*

By similar arguments as those in Lemma 3.4, we have

Lemma 4.4. *Let* $G \in \mathcal{B}_2(n)$*, where* $|\widehat{G}| \geq 11$*,* $G \neq B_n^2$ *and* $n \geq 12$*. Then* $G \prec B_n^2$*.*

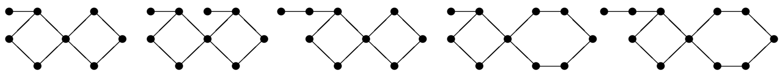
Combining Lemmas 4.1 and 4.4, and using the increasing property (2), we obtain the following theorem.

Theorem 4.1. *Let* $G \in \mathcal{B}_2(n)$*, where* $G \neq B_n^2$ *and* $n \geq 12$*. Then* $G \prec B_n^2$ *and* $E(G) < E(B_n^2)$*.*

Remark. Let $A_8^2, A_9^2, A_9^{2'}, A_{10}^2$ and A_{11}^2 be the graphs shown in Fig. 3. For $n = 8, 9, 10, 11$, we have

(i) if $G \in \mathcal{B}_2(n)$ with $G \neq A_n^2$, then $G \prec A_n^2$ and $E(G) < E(A_n^2)$, for $n = 8, 10, 11$,

(ii) if $G \in \mathcal{B}_2(9)$ with $G \neq A_9^2, A_9^{2'}$, then $G \prec A_9^2$ or $A_9^{2'}$, $E(A_9^{2'}) = 10.3376 < E(A_9^2) = 10.9418$, and so if $G \in \mathcal{B}_2(9)$ with $G \neq A_9^2$, then $E(G) < E(A_9^2)$.



$A_8^2\,(= B_{8,4}^4)$ $\quad A_9^2 \quad$ $A_9^{2'}\,(= B_{9,4}^4)$ $\quad A_{10}^2\,(= B_{10,4}^6)$ $\quad A_{11}^2\,(= B_{11,4}^6)$

Figure 3: Graphs with maximal energies and a related graph in $\mathcal{B}_2(n)$, where $n = 8, 9, 10, 11$.

5. GRAPHS IN $\mathcal{B}_3(n)$ WITH MAXIMAL ENERGY

Let $B'_{n,t}$ for $1 \leq t \leq n-13$ ($B''_{n,t}$ for $1 \leq t \leq n-12$, resp.) be the graph obtained by attaching a path P_t to vertex y (vertex w, resp.) in B_{n-t}^*, where y and w are neighbors of a vertex of degree 3 in B_{n-t}^* such that y lies outside any cycle and w lies on some cycle in B_{n-t}^*. Denote by $U_{n,t}^a$ be the graph obtained by attaching a path P_t to a vertex on the cycle that is adjacent to the vertex of degree 3 in P_{n-t}^a, where $1 \leq t \leq n-a-t$.

Lemma 5.1. *For* $n \geq 16$*,* $B'_{n,2} \prec B_n^3$*.*

Proof. By Lemma 2.1 (ii),

$$\begin{aligned} b_{2i}(B'_{n,2}) &= b_{2i}(P^6_{n,7,2}) + b_{2i-2}(P_4 \cup P^6_{n-6}) + 2b_{2i-6}(P^6_{n-6}), \\ b_{2i}(B^3_n) &= b_{2i}(P^6_{n,7,n-13}) + b_{2i-2}(P_4 \cup P^6_{n-6}) + 2b_{2i-6}(P^6_{n-6}). \end{aligned}$$

So, to prove $B'_{n,2} \prec B^3_n$, it suffices to prove $P^6_{n,7,2} \prec P^6_{n,7,n-13}$. By Lemma 2.1 (i),

$$\begin{aligned} b_{2i}(P^6_{n,7,2}) &= b_{2i}(P_6 \cup P^6_{n-6}) + b_{2i-2}(P_5 \cup P_2 \cup P^6_{n-9}), \\ b_{2i}(P^6_{n,7,n-13}) &= b_{2i}(P_6 \cup P^6_{n-6}) + b_{2i-2}(P_5 \cup P_{n-13} \cup C_6). \end{aligned}$$

By Lemma 2.7 (ii), $P_2 \cup P^6_{n-9} \prec P_{n-13} \cup C_6$ and so $P^6_{n,7,2} \prec P^6_{n,7,n-13}$. □

Similarly, we have

Lemma 5.2. *For $n \geq 15$, $B'_{n,1} \prec B^3_n$.*

Lemma 5.3. *For $n \geq 15$, $B''_{n,2} \prec B^3_n$.*

Proof. If $15 \leq n \leq 16$, then by direct checking (see Table 1), we have $B''_{n,2} \prec B^3_n$.

Suppose that $n \geq 17$. By Lemma 5.1, to prove $B''_{n,2} \prec B^3_n$, we need only to prove $B''_{n,2} \preceq B'_{n,2}$. By Lemmas 2.1 and 2.7 (iii),

$$\begin{aligned} b_{2i}(B''_{n,2}) &= b_{2i}(P_2 \cup B^*_{n-2}) + b_{2i-2}(P_1 \cup P^6_{n-3}) \\ &= b_{2i}(P_2 \cup B^*_{n-2}) + b_{2i-2}(P_{n-3}) + b_{2i-4}(P_4 \cup P_{n-9}) + 2b_{2i-8}(P_{n-9}) \\ &\leq b_{2i}(P_2 \cup B^*_{n-2}) + b_{2i-2}(P_{n-9} \cup C_6) + b_{2i-4}(P_4 \cup P_{n-15} \cup C_6) \\ &\quad +2b_{2i-8}(P_{n-15} \cup C_6) = b_{2i}(B'_{n,2}), \end{aligned}$$

implying $B''_{n,2} \preceq B'_{n,2}$. □

Similarly, we have

Lemma 5.4. *For $n \geq 14$, $B''_{n,1} \prec B^3_n$.*

By Lemma 2.1 (ii), we have $P^6_n \prec B^3_n$ for $n = 13$. By Lemmas 2.1 (ii) and 5.4, we have $P^6_n \prec B''_{n,1} \prec B^3_n$ for $n \geq 14$.

Lemma 5.5. *Let $G \in \mathcal{B}_3(n)$, where $|\widehat{G}| < 13$, $|\widehat{G}| \neq B^*_{12}$ and $n \geq 13$. Then $G \prec B^3_n$.*

Proof. Obviously, G contains at least one quadrangle. We prove the lemma by induction on n.

Suppose that $n = 13$. If each vertex of some quadrangle $v_1v_2v_3v_4v_1$ is not a branching vertex of G, then let $\deg_{\widehat{G}}(v_1) = 3$ and by Lemmas 2.1, 2.5 and 2.7 (i),

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G - v_1v_2 - v_2v_3) + b_{2i-2}(G - v_2 - v_3 - v_4v_1) \\ &\quad + b_{2i-2}(G - v_1 - v_2 - v_3v_4) \\ &\leq b_{2i}(P_1 \cup P_{12}^6) + b_{2i-2}(P_1 \cup P_{10}^6) + b_{2i-2}(P_1 \cup P_1 \cup P_9^6) \\ &\leq b_{2i}(P_{12}^6) + b_{2i-2}(P_{11}^6) + b_{2i-2}(P_4 \cup P_7^6) \\ &= b_{2i}(B_{13}^3) - 2b_{2i-6}(P_7^6). \end{aligned}$$

Hence, $G \preceq B_{13}^3$ and $b_6(G) < b_6(B_{13}^3)$, implying $G \prec B_{13}^3$.

Suppose that there exists at least one branching vertex in each quadrangle of G. If there exists exactly a branching vertex v on some quadrangle such that v has exactly one pendent neighbor outside $\widehat{G}$, then by similar arguments as above, we have $G \prec B_{13}^3$. Otherwise, there exists some edge zv in G such that $\deg_{\widehat{G}}(z) = 3$ and $G - zv$ contains exactly two vertex-disjoint bipartite unicyclic graphs, the one containing z possesses 6 vertices and the other possesses 7 vertices. By Lemmas 2.1 (i), 2.3 and 2.5,

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G - zv) + b_{2i-2}(G - z - v) \\ &\leq b_{2i}(C_6 \cup P_7^6) + b_{2i-2}(P_5 \cup C_6) = b_{2i}(B_{13}^3), \end{aligned}$$

Thus $G \preceq B_{13}^3$. Moreover $b_4(G) < b_4(B_{13}^3)$. So $G \prec B_{13}^3$.

Suppose that $n = 14$. Suppose that $d_G(u, \widehat{G}) = 1$ for some $u \in V_p(G)$. Then $G - u \in \mathcal{B}_3(13)$ and thus $G - u \prec B_{13}^3$. Let $v \in \Gamma_G(u)$. If v lies on some cycle, then by Lemma 2.5, $G - u - v \preceq P_{12}^6$. If v lies outside any cycle, then by Lemma 2.5, $G - u - v \preceq P_5^4 \cup P_7^6$, $C_4 \cup P_8^6$ or $C_6 \cup C_6$, and by Sachs theorem, P_{12}^6, $P_5^4 \cup P_7^6$, $C_4 \cup P_8^6$ $\preceq C_6 \cup C_6$. Therefore, by Lemma 2.9, $G \prec B_{14}^3$.

Suppose that $d_G(u, \widehat{G}) \geq 2$ for any $u \in V_p(G)$. Obviously, G have at most three branching vertices. If each vertex in some quadrangle is not a branching vertex of G, or there exist two quadrangles in which each contains exactly a branching vertex of G, then by similar arguments as above, $G \prec B_{14}^3$. Otherwise, $\widehat{G} = B_{10,4,6}^*$, the quadrangle in G has two branching vertices, and thus by Sachs theorem, $G \prec B_{14}^3$.

Suppose that $n \geq 15$, the result holds for $n-1$ and $n-2$, and $G \in \mathcal{B}_3(n)$. By similar arguments as those in Lemma 3.1, we have $G \prec B_n^3$. $\square$

Lemma 5.6. *Let $G \in \mathcal{B}_3(n)$, where $|\widehat{G}| = B_{12}^*$ and $n \geq 15$. Then $G \prec B_n^3$.*

Proof. By similar arguments as those in Lemma 3.1, we have $G \preceq B''_{n,n-12}$ for $G \in \mathcal{B}_3(n)$, where $|\widehat{G}| = B_{12}^*$ and $n \geq 13$. Now we show that $B''_{n,n-12} \prec B_n^3$ for $n \geq 15$. By Lemma 2.1 (i),

$$\begin{aligned} b_{2i}(B''_{n,n-12}) &= b_{2i}(C_6 \cup P_{n-6}^6) + b_{2i-2}(P_5 \cup P_{n-7}), \\ b_{2i}(B_n^3) &= b_{2i}(C_6 \cup P_{n-6}^6) + b_{2i-2}(P_5 \cup P_{n-13} \cup C_6). \end{aligned}$$

By Lemma 2.7 (iii), $P_{n-7} \prec P_{n-13} \cup C_6$. Thus $B''_{n,n-12} \prec B_n^3$. $\square$

Denote by $B'_{n,a,b}$ the bipartite bicyclic graph obtained from $B^*_{n-1,a,b}$ by attaching a pendent vertex to a vertex $w \in V(B^*_{n-1,a,b})$ with $d_{B^*_{n-1,a,b}}(w, C_a) = 1$, where $n \geq a+b+2$. For convenience, let $b \geq a$ if $n = a+b+2$.

Lemma 5.7. *For $a, b \geq 6$, $B'_{n,a,b} \preceq B'_{n,1}$.*

Proof. First, we show that $B'_{n,a,b} \preceq B'_{n,a,6}$ for $b \geq 8$. If $n > a+b+2$, then by Lemmas 2.1 (i) and 2.5,

$$b_{2i}(B'_{n,a,b}) \leq b_{2i}(C_a \cup P_{n-a}^6) + b_{2i-2}(P_{a-1} \cup P_{n-a-2}^6) = b_{2i}(B'_{n,a,6}).$$

Hence $B'_{n,a,b} \preceq B'_{n,a,6}$, in particular, $B'_{n,6,a} \preceq B'_{n,1}$.

Suppose that $n = a+b+2$. By Lemma 2.1,

$$\begin{aligned} b_{2i}(B'_{n,a,b}) &= b_{2i}(P^a_{n,b+1,1}) + b_{2i-2}(P_{b-2} \cup P^a_{a+2}) - (-1)^{\frac{b}{2}} 2b_{2i-b}(P^a_{a+2}) \\ &= b_{2i}(P^a_{n,b+1,1}) + b_{2i-2}(P_{b-2} \cup P^a_{a+1}) + b_{2i-4}(P_4 \cup P_{b-6} \cup C_a) \\ &\quad + b_{2i-6}(P_3 \cup P_{b-7} \cup C_a) - (-1)^{\frac{b}{2}} 2b_{2i-b}(P^a_{a+2}), \\ b_{2i}(B'_{n,a,6}) &= b_{2i}(P^a_{n,b+1,1}) + b_{2i-2}(P_4 \cup P^a_{n-6,b-5,1}) + 2b_{2i-6}(P^a_{n-6,b-5,1}) \\ &= b_{2i}(P^a_{n,b+1,1}) + b_{2i-2}(P_4 \cup P^a_{a+b-5}) + b_{2i-4}(P_4 \cup P_{b-6} \cup C_a) \\ &\quad + 2b_{2i-6}(P_{b-7} \cup P^a_{a+3,2,1}) + 2b_{2i-8}(P_{b-8} \cup P^a_{a+2}). \end{aligned}$$

By Lemma 2.2, $b_{2i-6}(P_3 \cup P_{b-7} \cup C_a) \leq b_{2i-6}(P_{b-7} \cup P^a_{a+3,2,1})$. To prove $B'_{n,a,b} \preceq B'_{n,a,6}$, we need only to prove

$$b_{2i-2}(P_{b-2} \cup P^a_{a+1}) \leq b_{2i-2}(P_4 \cup P^a_{a+b-5}) + b_{2i-6}(P_{b-7} \cup P^a_{a+3,2,1}).$$

By Lemmas 2.1, and 2.2,

$$\begin{aligned} b_{2i-2}(P_{b-2} \cup P^a_{a+1}) &= b_{2i-2}(P_4 \cup P_{b-6} \cup P^a_{a+1}) + b_{2i-4}(P_3 \cup P_{b-7} \cup C_a) \\ &\quad + b_{2i-6}(P_3 \cup P_{b-7} \cup P_{a-1}) \\ &\leq b_{2i-2}(P_4 \cup P_{b-6} \cup P^a_{a+1}) + b_{2i-4}(P_4 \cup P_{b-7} \cup C_a) \\ &\quad + b_{2i-6}(P_3 \cup P_{b-7} \cup C_a) \\ &\leq b_{2i-2}(P_4 \cup P^a_{a+b-5}) + b_{2i-6}(P_{b-7} \cup P^a_{a+3,2,1}). \end{aligned}$$

Next, we show that $B'_{n,a,6} \preceq B'_{n,6,a}$ for $a \geq 8$. By Lemma 2.1,

$$b_{2i}(B'_{n,a,6}) = b_{2i}(B^*_{n-1,a,6}) + b_{2i-2}(P_{n-a-8} \cup C_6 \cup C_a) + b_{2i-4}(P_{n-a-9} \cup P_5 \cup C_a),$$

$$b_{2i}(B'_{n,6,a}) = b_{2i}(B^*_{n-1,a,6}) + b_{2i-2}(P_{n-a-8} \cup C_a \cup C_6) + b_{2i-4}(P_{n-a-9} \cup P_{a-1} \cup C_6).$$

So, to prove $B'_{n,a,6} \preceq B'_{n,6,a}$, it suffices to prove $P_5 \cup C_a \preceq P_{a-1} \cup C_6$. By Lemma 2.1 (ii),

$$\begin{aligned} b_{2i}(P_5 \cup C_a) &= b_{2i}(P_5 \cup P_a) + b_{2i-2}(P_5 \cup P_{a-2}) - (-1)^{\frac{a}{2}} 2 b_{2i-a}(P_5), \\ b_{2i}(P_{a-1} \cup C_6) &= b_{2i}(P_6 \cup P_{a-1}) + b_{2i-2}(P_4 \cup P_{a-1}) + 2 b_{2i-6}(P_{a-1}). \end{aligned}$$

Since $b_{2i}(P_5 \cup P_a) \leq b_{2i}(P_6 \cup P_{a-1})$ and $b_{2i-2}(P_5 \cup P_{a-2}) \leq b_{2i-2}(P_4 \cup P_{a-1})$ by Lemma 2.6, we have $B'_{n,a,6} \preceq B'_{n,6,a}$.

Note that $B'_{n,6,a} \preceq B'_{n,1}$. The result follows. □

Let G be a bipartite bicyclic graph on $n \geq 16$ vertices and $G \neq B^*_{n,a,b}$, where $a, b \geq 10, a \equiv b \equiv 2 \pmod 4$ and $n = a + b$. Then [28] $G \preceq B^*_n$. By this result and by Sachs theorem for $13 \leq n \leq 15$, we have

Lemma 5.8. *Let G be a bipartite bicyclic graph on $n \geq 13$ vertices. If G contains two vertex-disjoint cycles but no pendent vertices, $G \neq B^*_{n,a,b}$, where $a, b \geq 10, a \equiv b \equiv 2 \pmod 4$ and $n = a + b$, then $G \preceq B^*_n$.*

Lemma 5.9. *Let $G \in \mathcal{B}_3(n)$, where $n = |\widehat{G}| + 2$, $|\widehat{G}| \geq 13$, $|V_p(G)| = 1$ and $G \neq B_n^3$. Then $G \prec B_n^3$.*

Proof. Let x be the unique pendent vertex of G. Let u the neighbor of x and v the unique branching vertex of G. Let C_a and C_b be the two vertex-disjoint cycles of G. Obviously, $n \geq 15$.

Case 1. $\widehat{G} = B^*_{n-2,a,b}$, where $a, b \geq 10, a \equiv b \equiv 2 \pmod 4$ and $n - 2 = a + b$.

Obviously, v lies on some cycle of G, say C_b, and $n = a + b + 2 \geq 22$. Take a vertex $w \in V(B^*_{n-2,a,b})$ with $d_{\widehat{G}}(w, C_a) = 2$. It is not difficult to show that $G \preceq G'$, where G' is obtained from G by removing edge uv and adding edge uw. By Lemma 5.1, to prove $G' \prec B_n^3$, we need only to prove $G' \preceq B'_{n,2}$. By Lemmas 2.1 (ii) and 2.5,

$$\begin{aligned} b_{2i}(G') &= b_{2i}(U^b_{n,2}) + b_{2i-2}(P_{a-2} \cup P^b_{n-a}) + 2b_{2i-a}(P^b_{n-a}) \\ &\leq b_{2i}(U^b_{n,2}) + b_{2i-2}(P_{a-2} \cup P^6_{n-a}) + 2b_{2i-a}(P^6_{n-a}), \\ b_{2i}(B'_{n,2}) &= b_{2i}(P^6_{n,7,2}) + b_{2i-2}(P_4 \cup P^6_{n-6}) + 2b_{2i-6}(P^6_{n-6}). \end{aligned}$$

By Lemma 2.7 (i), $b_{2i-2}(P_{a-2} \cup P^6_{n-a}) \leq b_{2i-2}(P_4 \cup P^6_{n-6})$, and by Lemma 2.1 (i), $b_{2i-a}(P^6_{n-a}) \leq b_{2i-6}(P^6_{n-6})$. To prove $G' \preceq B'_{n,2}$, it suffices to prove $U^b_{n,2} \preceq P^6_{n,7,2}$. By Lemmas 2.1 and 2.5,

$$\begin{aligned} b_{2i}(U^b_{n,2}) &= b_{2i}(P_n) + b_{2i-2}(P_2 \cup P_{n-b-2} \cup P_{b-2}) + 2b_{2i-b}(P_2 \cup P_{n-b-2}) \\ &= b_{2i}(P_2 \cup P_{n-2}) + b_{2i-2}(P_6 \cup P_{n-9}) + b_{2i-2}(P_2 \cup P_{n-b-2} \cup P_{b-2}) \\ &\quad + b_{2i-4}(P_4 \cup P_5 \cup P_{n-14}) + b_{2i-6}(P_3 \cup P_5 \cup P_{n-15}) \\ &\quad + 2b_{2i-b}(P_2 \cup P_{n-b-2}), \\ b_{2i}(P^6_{n,7,2}) &= b_{2i}(P_{n,7,2}) + b_{2i-2}(P_4 \cup P_{n-6,7,2}) + 2b_{2i-6}(P_{n-6,7,2}), \\ &= b_{2i}(P_2 \cup P_{n-2}) + b_{2i-2}(P_6 \cup P_{n-9}) + b_{2i-2}(P_2 \cup P_4 \cup P_{n-8}) \\ &\quad + b_{2i-4}(P_4 \cup P_6 \cup P_{n-15}) + 2b_{2i-6}(P_{n-7,7,2}) + 2b_{2i-8}(P_{n-8,7,2}). \end{aligned}$$

By Lemma 2.6, $b_{2i-2}(P_2 \cup P_{n-b-2} \cup P_{b-2}) \leq b_{2i-2}(P_2 \cup P_4 \cup P_{n-8})$ and $b_{2i-4}(P_4 \cup P_5 \cup P_{n-14}) \leq b_{2i-4}(P_4 \cup P_6 \cup P_{n-15})$. By Lemmas 2.2 and 2.6, $b_{2i-6}(P_3 \cup P_5 \cup P_{n-15}) \leq b_{2i-6}(P_2 \cup P_{n-9}) \leq b_{2i-6}(P_{n-7,7,2})$. Note that $b_{2i-b}(P_2 \cup P_{n-b-2}) \leq b_{2i-8}(P_{n-8,7,2})$. We have $U^b_{n,2} \preceq P^6_{n,7,2}$.

Case 2. $\widehat{G} \neq B^*_{n-2,a,b}$, where $a, b \geq 10, a \equiv b \equiv 2 \pmod 4$ and $n - 2 = a + b$.

Subcase 2.1. v lies on some cycle of G.

By Lemma 5.3, to prove $G \prec B^3_n$, we need only to prove $G \preceq B''_{n,2}$. Clearly, $G - x - u$ is a bicyclic graph containing no pendent vertices and $G - x - u - v$ is a bipartite graph on $n - 3$ vertices containing a unique cycle. Then by Lemma 5.8, $G - x - u \preceq B^*_{n-2}$, and by Lemma 2.5, $G - x - u - v \preceq P^6_{n-3}$. Thus, by Lemma 2.9, $G \preceq B''_{n,2}$.

Subcase 2.2. v lies outside any cycle of G.

Suppose that there exists some quadrangle $v_1v_2v_3v_4v_1$ in G with $\deg_{\widehat{G}}(v_1) = 3$. Then by Lemmas 2.1, 2.5 and 2.7 (i) and (ii),

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G - v_1v_2 - v_2v_3) + b_{2i-2}(G - v_2 - v_3 - v_4v_1) \\ &\quad + b_{2i-2}(G - v_1 - v_2 - v_3v_4) \\ &\leq b_{2i}(P_1 \cup P^6_{n-1}) + b_{2i-2}(P_1 \cup P^6_{n-3}) + b_{2i-2}(P_1 \cup P_1 \cup P^6_{n-4}) \\ &\leq b_{2i}(P^6_{n-1}) + b_{2i-2}(P_{n-8} \cup C_6) + b_{2i-2}(P_4 \cup P^6_{n-7}) \\ &= b_{2i}(B'_{n,1}) - b_{2i-4}(P_4 \cup P_{n-14} \cup C_6) - 2b_{2i-6}(P^6_{n-6,n-13,1}). \end{aligned}$$

Hence $G \preceq B'_{n,1}$. By Lemma 5.2, $B'_{n,1} \prec B^3_n$. Thus $G \prec B^3_n$.

Suppose that G contains no quadrangles. Since $G \neq B^3_n$, we have $n \geq 16$. By Lemma 5.1, to prove $G \prec B^3_n$, it suffices to prove $G \preceq B'_{n,2}$. Clearly, $G - x \in \mathcal{B}_3(n-1)$ contains exactly one pendent vertex and $G - x - u$ is a bicyclic graph containing no pendent vertices, and by Lemma 5.8, $G - x - u \preceq B^*_{n-2}$. By Lemma 2.9, we need only to prove $G - x \preceq B'_{n-1,1}$. If $G - x = B'_{n-1,a,b}$, then by Lemma 5.7, $G - x \preceq B'_{n-1,1}$. Otherwise, all neighbors of v lie outside any cycle of G. Then $G - x - u - v = P^a_t \cup P^b_s$, where $t > a$, $s > b$ and $n = t + s + 3$, and thus by Lemmas 2.5 and 2.8, $G - x - u - v \preceq C_6 \cup P^6_{n-9}$. Note that $G - x - u \preceq B^*_{n-2}$. Hence, by Lemma 2.9, $G - x \preceq B'_{n-1,1}$. □

Similarly, we have

Lemma 5.10. *Let $G \in \mathcal{B}_3(n)$, where $n = |\widehat{G}| + 1$, $|\widehat{G}| \geq 13$ and $G \neq B^3_n$. Then $G \prec B^3_n$.*

By similar arguments as those in Lemma 3.4, we have

Lemma 5.11. *Let $G \in \mathcal{B}_3(n)$, where $|\widehat{G}| \geq 13$, $G \neq B_n^3$ and $n \geq 14$. Then $G \prec B_n^3$.*

Combining Lemmas 5.5, 5.6 and 5.11, and using the increasing property (2), we have the following theorem.

Theorem 5.1. *Let $G \in \mathcal{B}_3(n)$, where $G \neq B_n^3$ and $n \geq 15$. Then $G \prec B_n^3$ and $E(G) < E(B_n^3)$.*

Remark. Let $A_9^3, A_{10}^3, A_{10}^{3'}, A_{10}^{3''}, A_{11}^3, A_{12}^3$ and $A_{12}^{3'}$ be the graphs shown in Fig. 4. Let $A_{13}^3 = B''_{13,1}$ and $A_{14}^3 = B''_{14,2}$. For $n = 9, 10, 11, 12, 13, 14$, we have

(i) if $G \in \mathcal{B}_3(n)$ with $G \neq A_n^3$, then $G \prec A_n^3$ and $E(G) < E(A_n^3)$, for $n = 9, 11, 13, 14$,

(ii) if $G \in \mathcal{B}_3(10)$ with $G \neq A_{10}^3, A_{10}^{3'}, A_{10}^{3''}$, then $G \prec A_{10}^3, A_{10}^{3'}$ or $A_{10}^{3''}$, $E(A_{10}^{3'}) = 11.8641 < E(A_{10}^{3''}) = 11.9315 < E(A_{10}^3) = 12.4709$ and so if $G \in \mathcal{B}_3(10)$ with $G \neq A_{10}^3$, then $E(G) < E(A_{10}^3)$,

(iii) if $G \in \mathcal{B}_3(12)$ with $G \neq A_{12}^3, A_{12}^{3'}$, then $G \prec A_{12}^3$ or $A_{12}^{3'}$, $E(A_{12}^{3'}) = 15.1349 < E(A_{12}^3) = 15.6722$, and so if $G \in \mathcal{B}_3(12)$ with $G \neq A_{12}^3$, then $E(G) < E(A_{12}^3)$.

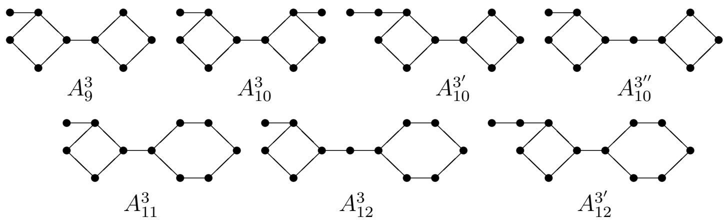


Figure 4: Graphs with maximal energies and related graphs in $\mathcal{B}_3(n)$, where $n = 9, 10, 11, 12$.

6. COMMENTS

We have determined the graphs in $\mathcal{B}_i(n)$ for $i = 1, 2, 3$ with maximal energies above. Now we determine the graphs with maximal energy in the class of bipartite bicyclic graphs with exactly two cycles and at least one pendent vertex.

Theorem 6.1. *Let $G \in \mathcal{B}_2(n) \cup \mathcal{B}_3(n)$, where $G \neq B_n^3$ and $n \geq 15$. Then $G \prec B_n^3$ and $E(G) < E(B_n^3)$.*

Proof. By Theorems 4.1 and 5.1, and using the increasing property (2), it suffices to show $B_n^2 \prec B_n^3$. We prove this by induction on n. By direct checking (see Table 1), the result holds for $n = 15$ and $n = 16$.

Suppose that $n \geq 17$, the result holds for $n-1$ and $n-2$, and $G \in \mathcal{B}(n) \backslash \mathcal{B}_1(n)$. By Lemma 2.1 (i), $b_{2i}(B_n^k) = b_{2i}(B_{n-1}^k) + b_{2i-2}(B_{n-2}^k)$, where $k = 2, 3$. Hence, by the induction hypothesis, $B_n^2 \prec B_n^3$. □

Remark. For $15 \leq n \leq 18$, by direct calculation of the eigenvalues, we find $E(B_n^1) < E(B_n^3)$, which can not be deduced by use of the relation "$\prec$" from the b_{2i}-values. This may be seen from Table 1 for $n = 15, 16$.

Table 1: b_{2i}-values and energies of some graphs

graph	coefficients							energy
	b_4	b_6	b_8	b_{10}	b_{12}	b_{14}	b_{16}	
B_{15}^1	100	317	550	520	245	43		19.7780
B_{15}^2	99	308	519	470	207	32		19.6188
B_{15}^3	100	316	549	532	270	56		19.8698
$B''_{15,2}$	100	315	541	507	240	44		19.7684
B_{16}^1	115	403	794	887	531	143	9	21.2109
B_{16}^2	114	393	755	813	460	111	4	20.9728
B_{16}^3	115	402	791	893	557	168	16	21.3495
$B''_{16,2}$	115	401	784	872	530	156	16	21.3219

Acknowledgement. This work was supported by the National Natural Science Foundation of China (Grant No. 10671076).

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