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On bicyclic graphs with maximal energy ☆

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Abstract

Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of a graph G of order n. The energy of G is defined as $E(G) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|$. Let $P_n^{6,6}$ be the graph obtained from two copies of C_6 joined by a path P_{n-10}, $\mathscr{B}_n$ be the class of all bipartite bicyclic graphs that are not the graph obtained from two cycles C_a and C_b ($a, b \geqslant 10$ and $a \equiv b \equiv 2 \pmod 4$) joined by an edge. In this paper, we show that $P_n^{6,6}$ is the graph with maximal energy in $\mathscr{B}_n$, which gives a partial solution to Gutman's conjecture in Gutman and Vidović (2001) [I. Gutman, D. Vidović, Quest for molecular graphs with maximal energy: a computer experiment, J. Chem. Inf. Sci. 41 (2001) 1002–1005].

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1. Introduction

Given a graph G (without loops and multiple edges) of n vertices labeled by $1, 2, \ldots, n$. We can form the adjacency matrix $A(G) = (a_{ij})_{n\times n}$ of G, defined by $a_{ij} = 1$ if v_i and v_j are adjacent, $a_{ij} = 0$ otherwise. The adjacency matrix depends on the labeling of the vertices but its characteristic equation depend only on the graph G itself. As $A(G)$ is a symmetric matrix, these eigenvalues of $A(G)$, called the eigenvalues of G, are real.

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We denote by $\phi(G, x)$ the characteristic polynomial $\det(xI - A(G))$ of G. It is well known [1] that if G is a bipartite graph, then

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

where $b_{2i}(G) = (-1)^i a_{2i}$ and $b_{2i}(G) \geqslant 0$ for all $i = 1, \ldots, \lfloor \frac{n}{2} \rfloor$. Clearly, $b_0(G) = 1$ and $b_2(G)$ equals the number of edges of G.

In chemistry, the experimental heats from the formation of conjugated hydrocarbons are closely related to the total π-electron energy. And the calculation of the total energy of all π-electrons in conjugated hydrocarbons can be reduced to (within the framework of HMO approximation) [3] that of

$$E = E(G) = \sum_{i=0}^{n} |\lambda_i|, \tag{1}$$

where λ_i are the eigenvalues of the corresponding graph G. The right-hand side of Eq. (1) is defined for all graphs (no matter whether they represent the carbon-atom skeleton of a conjugated electron system or not). In view of this, if G is any graph, then by means of Eq. (1) one defines $E(G)$ and calls it the energy of the graph G.

It is known [3] that for bipartite graph G,$E(G)$ can be also expressed as the Coulson integral formula

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

If for two bipartite graphs G_1 and G_2, $b_{2i}(G_1) \leqslant b_{2i}(G_2)$ holds for all $i = 1, 2, \ldots, \lfloor n/2 \rfloor$, we say that G_1 is smaller than G_2, and write $G_1 \preceq G_2$ or $G_2 \succeq G_1$. Moreover, if $b_{2i}(G_1) < b_{2i}(G_2)$ holds for some i, we write $G_1 \prec G_2$ or $G_2 \succ G_1$. From Eq.(2) we know that for two bipartite graphs G_1 and G_2

$$G_1 \preceq G_2 \Rightarrow E(G_1) \leqslant E(G_2), \quad G_1 \prec G_2 \Rightarrow E(G_1) < E(G_2).$$

If a graph G has n vertices, then we say that G is an n-graph; if G has n vertices and m edges, then it is referred to as an (n, m)-graph. Especially, we call a connected graph with n vertices a tree if it has $n - 1$ edges, a unicyclic graph if it has n edges, and a bicyclic graph if it has $n + 1$ edges. If G is a tree on n vertices, Gutman [2,5] showed that $E(S_n) \leqslant E(G) \leqslant E(P_n)$, where S_n, P_n denote the star and path with n vertices and they reach the respondence equalities, respectively. Let S_n^3 be the graph obtained from the star graph with n vertices by adding an edge, P_n^6 be the graph obtained by connecting a vertex of the cycle C_6 with a terminal vertex of the path P_{n-6}. Hou [6] showed that S_n^3 is the graph with minimal energy in all unicyclic graphs; In [7], Hou et al. showed that P_n^6 is the graph with maximal energy in all bipartite unicyclic graphs except C_n.

Let $S_n^{3,3}$ be the graph formed by joining $n - 4$ pendant vertices to a vertex of degree three of the graph $K_4 - e$, $P_n^{6,6}$ be the graph obtained from two copies of C_6 joined by a path of order $n - 10$ (see Fig. 1). Let $G(n)$ be the set of bicyclic graphs on n vertices and containing no disjoint odd cycles of lengths k and l with $k + l \equiv 2 \pmod 4$. The authors of [10] proved that $S_n^{3,3}$ is the graph with minimal energy in $G(n)$.

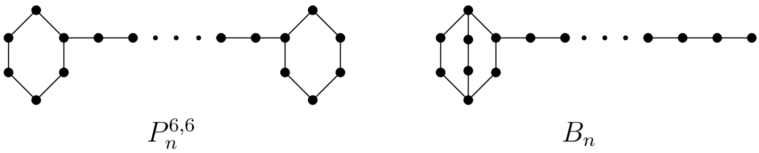

Fig. 1. Graphs $P_n^{6,6}$ and B_n.

About the bicyclic graphs with maximal energy Gutman proposed the following conjecture [4]:

Conjecture 1. *For $n = 14$ and $n \geqslant 16$ the bicyclic molecular graph of order n with maximal energy is the molecular graph of the α, β diphenyl-polyene $C_6H_5(CH)_{n-12}C_6H_5$, or denoted by $P_n^{6,6}$.*

Let $\mathscr{B}_n$ be the class of all bipartite bicyclic graphs that are not the graph obtained from two cycles C_a and C_b ($a, b \geqslant 10$ and $a \equiv b \equiv 2 \pmod 4$) joined by an edge. In this paper, we show that $P_n^{6,6}$ is the graph with maximal energy in $\mathscr{B}_n$.

Let P_n^a be the unicyclic graph obtained by connecting a vertex of C_a with a terminal vertex of P_{n-a}, $C(n; a, s, t)$ be the unicyclic graph obtained by attaching a pendant vertex of P_{t+1} to the $(s+1)$-th vertex of $P_{n-a-t+1}$ in P_{n-t}^a, and $P(n; s, t)$ be the tree obtained by attaching a pendant vertex of P_{t+1} to the $(s+1)$-th vertex of P_{n-t} (see Fig. 2). Following results are applied in the proof of our result:

If T is a tree with n vertices and not isomorphic to P_n, $P(n; 2, 2)$, then $P(n; 2, 2) \succ T$ (see [3]).

Let $U(n, a)$ be the set of all unicyclic graphs obtained from C_a by adding to it $n - a$ pendant vertices.

If $G \notin U(n, a) (a \equiv 0 (\mathrm{mod}\, 4))$ is a unicyclic graph and C_a is the unique cycle in G, then $G \preceq P_n^a$.

If $C_a (a \equiv 2 (\mathrm{mod}\, 4))$ is the unique cycle of unicyclic graph G, then $G \preceq P_n^a$ (see [8]).

In order to obtain the result we need some auxiliary lemmas.

Lemma 1 [1]. *Let uv be an edge of G, then*

$$\phi(G, \lambda) = \phi(G - uv, \lambda) - \phi(G - u - v, \lambda) - 2 \sum_{C \in \mathscr{C}(uv)} \phi(G - C, \lambda),$$

where $\mathscr{C}(uv)$ is the set of cycles containing uv.

In particular, if uv is a pendant edge of G with the pendant vertex v, then

$$\phi(G, \lambda) = \lambda\phi(G - v, \lambda) - \phi(G - u - v, \lambda).$$

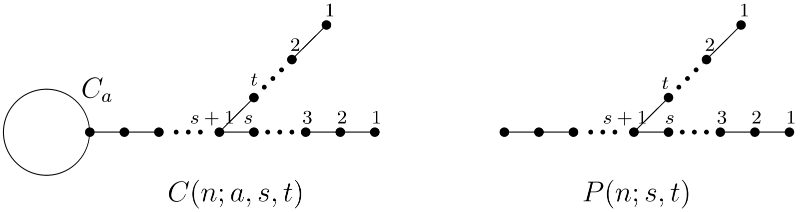

Fig. 2. Graphs $C(n;a,s,t)$ and $P(n;s,t)$.

Lemma 2 [9]. *Let uv be an edge of a bipartite bicyclic graph G, then*

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

where $\mathscr{C}(uv)$ is the set of cycles containing uv.

In particular, if uv is a pendant edge of G with the pendant vertex v, then

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

Proof. By Lemma 1, we have

$$a_{2i}(G) = a_{2i}(G - uv) - a_{2i-2}(G - u - v) - 2 \sum_{C_l \in \mathscr{C}(uv)} a_{2i-l}(G - C_l)$$

and

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

Since $b_{2i}(G) = (-1)^i a_{2i}(G)$ and G has at most two cycles containing uv, the result follows. □

Let G be a graph with characteristic polynomial $\phi(G, \lambda) = \sum_{i=0}^{n} a_i \lambda^{n-i}$. Then for $i \geqslant 1$

$$a_i = \sum_{S \in L_i} (-1)^{p(S)} 2^{c(S)},$$

where L_i denotes the set of Sachs graphs of G with i vertices, that is, the graphs in which every component is either a K_2 or a cycle, $p(S)$ is the number of components of S and $c(S)$ is the number of cycles contained in S. In addition, $a_0 = 1$. It is called Sachs Theorem (see [1]). From Sachs theorem we can obtain the following propositions for bipartite graphs:

1. If G_1 and G_2 are all bipartite graphs, then $b_{2k}(G_1 \cup G_2) = \sum_{i=0}^{k} b_{2i}(G_1) \cdot b_{2k-2i}(G_2)$;
2. Let G, $G + e$ be all bipartite graphs, where $e \notin E(G)$ and $G + e$ denotes the graph obtained from G by adding the edge e to it. If either the length of any cycle containing e equals 2 (mod 4) or e is not contained in any cycle, then $G \preceq G + e$;
3. If G_0, G_1, G_2 are all bipartite and $G_1 \preceq G_2$, since $b_{2i}(G_0) \geqslant 0$ and $b_{2i}(G_1) \leqslant b_{2i}(G_2)$ for all positive integer i, we have $G_0 \cup G_1 \preceq G_0 \cup G_2$. Moreover, for bipartite graphs G_i, G_i', if G_i has the same order as G_i' and $G_i \preceq G_i'$ for$i = 1, 2$, then $G_1 \cup G_2 \preceq G_1' \cup G_2'$.

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

$$P_n \succ P_2 \cup P_{n-2} \succ P_4 \cup P_{n-4} \succ \ldots \succ P_{2k} \cup P_{n-2k} \succ P_{2k+1} \cup P_{n-2k-1} \succ P_{2k-1} \cup P_{n-2k+1} \succ \ldots \succ P_3 \cup P_{n-3} \succ P_1 \cup P_{n-1}.$$

2. Main result

Let $\mathscr{B}_n$ be defined as above, $\mathscr{B}_n^1$, a subset of $\mathscr{B}_n$, all graphs with exact two edge-disjoint cycles, and $\mathscr{B}_n^2 = \mathscr{B}_n \setminus \mathscr{B}_n^1$, all graphs with exact three cycles.

Lemma 4. *Let* $G \in \mathscr{B}_n^1$ $(n \geqslant 16)$ *and* $G \ncong P_n^{6,6}$, *then* $G \prec P_n^{6,6}$.

Proof. Since $G \in \mathscr{B}_n^1$, G contains exactly two cycles, say C_a and C_b, that are connected by a path $P_t(t \geqslant 1)$. This subgraph is called the *center construct* of G, denoted by $\Theta(a, b; t)$. In this way, G is also viewed as the graph obtained from $\Theta(a, b; t)$ by planting some trees on it.

Case 1. $t \geqslant 2$.

Subcase 1.1. There is not an edge uv of P_t such that $G - uv$ contains two components whose orders are of at least 6. Then G contains the center construct $\Theta(4, a; 2)$ (or $\Theta(4, a; 3)$) and there is at most one edge planted on the C_4 of $\Theta(4, a; 2)$(or no tree is planted on C_4 of $\Theta(4, a; 3)$).

If G contains $\Theta(4, a; 2)$ and no tree is planted on the C_4, let uv be an edge of C_a and u be the vertex of degree 3 in $\Theta(4, a; 2)$. By Lemma 2 we have

$$b_{2i}(G) = b_{2i}(G - uv) + b_{2i-2}(G - u - v) + (-1)^{1+\frac{a}{2}} 2b_{2i-a}(G - C_a)$$
$$b_{2i}(P_n^{6,6}) = b_{2i}(P_n^6) + b_{2i-2}(P_{n-6}^6 \cup P_4) + 2b_{2i-6}(P_{n-6}^6).$$

From [7] we know that $P_n^6 \succ G - uv$ and $b_{2i-6}(P_{n-6}^6) > b_{2i-6}(P_{n-6}^4) > b_{2i-8}(P_{n-8}^4) > \cdots > b_{2i-a}(G - C_a)$ for $a \equiv 2 \pmod 4$. If $a \equiv 0 \pmod 4$, the result is obvious.

It suffices to prove that $G - u - v \prec P_{n-6}^6 \cup P_4$. Clearly, $G - u - v \prec C_4 \cup P_{n-6}$. By Lemma 2 we have

$$\begin{aligned}
b_{2k}(G - u - v) &\leqslant b_{2k}(P_4 \cup P_{n-6}) + b_{2k-2}(P_2 \cup P_{n-6}) - 2b_{2k-4}(P_{n-6}) \\
&= b_{2k}(P_4 \cup P_{n-6}) + b_{2k-2}(P_2 \cup P_4 \cup P_{n-10}) \\
&\quad + b_{2i-4}(P_2 \cup P_3 \cup P_{n-11}) - 2b_{2k-4}(P_{n-6}) \\
&\leqslant b_{2k}(P_4 \cup P_{n-6}) + b_{2k-2}(P_2 \cup P_4 \cup P_{n-10}) - b_{2k-4}(P_{n-6}) \\
&\leqslant b_{2k}(P_4 \cup P_{n-6}) + b_{2k-2}(2P_2 \cup P_4 \cup P_{n-12}) \\
&\quad + b_{2i-4}(P_2 \cup P_4 \cup P_1 \cup P_{n-13}) - b_{2k-4}(P_{n-6}) \\
&< b_{2k}(P_4 \cup P_{n-6}) + b_{2k-2}(P_4 \cup P_4 \cup P_{n-12}) + 2b_{2k-6}(P_4 \cup P_{n-12}) \\
&= b_{2k}(P_{n-6}^6 \cup P_4).
\end{aligned}$$

If G contains $\Theta(4, a; 2)$ and only one pendant edge is planted on the C_4, or G contains $\Theta(4, a; 3)$ and no tree is planted on the C_4, similar to the above proof we can also prove $G \prec P_n^{6,6}$.

Subcase 1.2. There exists an edge uv of P_t such that $G - uv$ contains two components with orders at least 6.

If there is at least one cycle C_4, suppose that G is the graph obtained from $\Theta(4, a, t)$ by planting some trees on it and uv be an edge of C_a that is incident to P_t. By Lemma 2 we have

$$b_{2i}(G) = b_{2i}(G - uv) + b_{2i-2}(G - u - v) + (-1)^{1+\frac{a}{2}} 2b_{2i-a}(G - C_a),$$
$$b_{2i}(P_n^{6,6}) = b_{2i}(P_n^6) + b_{2i-2}(P_{n-6}^6 \cup P_4) + 2b_{2i-6}(P_{n-6}^6).$$

Similar to above discussion, it suffices to prove $b_{2i-2}(G - u - v) < b_{2i-2}(P_{n-6}^6 \cup P_4)$. Since the component containing C_4 in $G - u - v$ has at least 6 vertices and $a \geqslant 4$, we write the component $G_x (x \geqslant 6)$. From Lemma 2 of [8] we have $G_x \preceq P_x^4$ (or $G_x \in U(x, 4)$, the proof of this case is similar). it is reduced to the following claim:

Claim 1. *$P^4_{n-x} \cup P_x \preceq P^4_{n-2} \cup P_2 \prec P^6_{n-4} \cup P_4$, where $n-x \geqslant 6$ and $x \geqslant 1$.*

Proof. Deleting the edge of P_{n-x-3} that is incident to C_4 in $P^4_{n-x} \cup P_x$ and the edge of P_{n-5} that is incident to C_4 in $P^4_{n-2} \cup P_2$, and Combining Lemmas 2 and 3 we can obtain the first inequality.

By Lemma 2 we have

$$\begin{aligned} b_{2i}(P^4_{n-2} \cup P_2) &= b_{2i}(P_{n-2} \cup P_2) + b_{2i-2}(2P_2 \cup P_{n-6}) - 2b_{2i-4}(P_{n-6} \cup P_2) \\ &= b_{2i}(2P_2 \cup P_{n-4}) + b_{2i-2}(2P_2 \cup P_{n-6}) + b_{2i-2}(P_1 \cup P_2 \cup P_{n-5}) \\ &\quad - 2b_{2i-4}(P_{n-6} \cup P_2) \\ &< b_{2i}(2P_2 \cup P_{n-4}) + b_{2i-2}(2P_2 \cup P_4 \cup P_{n-10}) + b_{2i-2}(3P_1 \cup P_{n-5}) \\ &< b_{2i}(2P_2 \cup P_{n-4}) + b_{2i-2}(2P_1 \cup P_{n-4}) + b_{2i-2}(2P_4 \cup P_{n-10}) \\ &\quad + 2b_{2i-6}(P_4 \cup P_{n-10}) \\ &= b_{2i}(P_4 \cup P_{n-4}) + b_{2i-2}(2P_4 \cup P_{n-10}) + 2b_{2i-6}(P_4 \cup P_{n-10}) \\ &= b_{2i}(P^6_{n-4} \cup P_4). \end{aligned}$$

Thus we complete the proof of the claim. □

In the following cases we assume that G contains two cycles C_a and C_b $(a, b \geqslant 6)$.

Subcase 1.2.1. $G \cong \Theta(a, b; 2)(a, b \geqslant 6)$. Thus $n = a + b$.

If there is a cycle of length 6, then $a \geqslant 10$. Let xy be an edge of C_a that is incident to the P_2 of $\Theta(a, 6; 2)$. By Lemma 2 we have

$$\begin{aligned} &b_{2i}(G) = b_{2i}(P^6_n) + b_{2i-2}(C_6 \cup P_{n-8}) + (-1)^{1+\frac{a}{2}} 2b_{2i-a}(C_6) \\ &b_{2i}(P^{6,6}_n) = b_{2i}(P^6_n) + b_{2i-2}(P^6_{n-6} \cup P_4) + 2b_{2i-6}(P^6_{n-6}). \end{aligned}$$

It suffices to prove

$$b_{2i-2}(P^6_{n-6} \cup P_4) + 2b_{2i-6}(P^6_{n-6}) \geqslant b_{2i-2}(C_6 \cup P_{n-8}) + (-1)^{1+\frac{a}{2}} 2b_{2i-a}(C_6).$$

By Sachs Theorem we have that for $i = 1, 2, 3$

$$\begin{aligned} &b_{2i-2}(P^6_{n-6} \cup P_4) + 2b_{2i-6}(P^6_{n-6}) = 1, n-3, n^2 - 9n + 24, \\ &b_{2i-2}(C_6 \cup P_{n-8}) + (-1)^{1+\frac{a}{2}} 2b_{2i-a}(C_6) = 1, n-3, n^2 - 9n + 20. \end{aligned}$$

Assuming $i \geqslant 4$, we have

$$\begin{aligned} b_{2i-2}(C_6 \cup P_{n-8}) &= b_{2i-2}(P_6 \cup P_{n-8}) + b_{2i-4}(P_4 \cup P_{n-8}) \\ &\quad + 2b_{2i-8}(P_4 \cup P_{n-12}) + 2b_{2i-10}(P_3 \cup P_{n-13}) \\ b_{2i-2}(P^6_{n-6} \cup P_4) &= b_{2i-2}(P_{n-6} \cup P_4) + b_{2i-4}(2P_4 \cup P_{n-12}) \\ &\quad + 2b_{2i-8}(P_{n-12} \cup P_4) \end{aligned}$$

and

$$\begin{aligned} 2b_{2i-6}(P^6_{n-6}) &= 2b_{2i-6}(P_{n-6}) + 2b_{2i-8}(P_4 \cup P_{n-12}) + 4b_{2i-12}(P_{n-12}) \\ &= b_{2i-6}(P_4 \cup P_3 \cup P_{n-13}) + b_{2i-8}(P_3 \cup P_{n-11}) \end{aligned}$$

$$+b_{2i-8}(P_4 \cup P_2 \cup P_{n-14}) + b_{2i-6}(P_{n-6})$$
$$+2b_{2i-8}(P_4 \cup P_{n-12}) + 4b_{2i-12}(P_{n-12}).$$

Since

$$b_{2i-4}(P_4 \cup P_{n-8}) = b_{2i-4}(2P_4 \cup P_{n-12}) + b_{2i-6}(P_4 \cup P_3 \cup P_{n-13})$$
$$b_{2i-8}(P_3 \cup P_{n-11}) = b_{2i-8}(P_1 \cup P_3 \cup P_{n-12}) + b_{2i-10}(P_3 \cup P_{n-13})$$
$$b_{2i-8}(P_4 \cup P_2 \cup P_{n-14}) = b_{2i-8}(P_4 \cup 2P_1 \cup P_{n-14}) + b_{2i-10}(P_4 \cup P_{n-14}),$$

we have

$$\begin{aligned} b_{2i-2}(P_{n-6}^6 \cup P_4) + 2b_{2i-6}(P_{n-6}^6) \geqslant\ & b_{2i-2}(C_6 \cup P_{n-8}) + b_{2i-8}(P_1 \cup P_3 \cup P_{n-12}) \\ & + b_{2i-8}(P_4 \cup 2P_1 \cup P_{n-14}) + b_{2i-6}(P_{n-6}) \\ & + 2b_{2i-8}(P_4 \cup P_{n-12}) + 4b_{2i-12}(P_{n-12}). \end{aligned}$$

For $a \equiv 0 \pmod 4$ the result is obvious, we thus assume $a \equiv 2 \pmod 4$ and since $2b_{2i-a}(C_6) = 0$ for $2i < a$, $2b_{2i-a}(C_6) = 2$ for $2i = a$, $2b_{2i-a}(C_6) = 12$ for $2i = a + 2$, $2b_{2i-a}(C_6) = 18$ for $2i = a + 4$, and $2b_{2i-a}(C_6) = 8$ for $2i = a + 6 = n$. By simple computation we have

$$b_{2i-2}(P_{n-6}^6 \cup P_4) + 2b_{2i-6}(P_{n-6}^6) > b_{2i-2}(C_6 \cup P_{n-8}) + (-1)^{1+\frac{a}{2}} 2b_{2i-a}(C_6).$$

If there is a cycle of length 0 (mod 4), say $b \equiv 0 \pmod 4$, thus $b \geqslant 8$. Similarly, we have

$$b_{2i}(G) = b_{2i}(P_n^a)) + b_{2i-2}(C_a \cup P_{b-2}) - 2b_{2i-b}(C_a).$$

Deleting an edge of C_a in $C_a \cup P_{b-2}$ and an edge of C_6 in $C_6 \cup P_{n-8}$, and applying Lemma 3, we can prove $C_6 \cup P_{n-8} \succ C_a \cup P_{b-2}$. Thus, we also have

$$b_{2i-2}(P_{n-6}^6 \cup P_4) + 2b_{2i-6}(P_{n-6}^6) > b_{2i-2}(C_6 \cup P_{n-8}) > b_{2i-2}(C_a \cup P_{b-2}),$$

and $P_n^a \prec P_n^6$, we complete the proof of the subcase.

Subcase 1.2.2: $t \geqslant 6$. We can choose an edge rs of P_t such that $G - rs$ and $G - r - s$ contain two components of orders at least 6 that are either unicyclic graphs or trees and each component is not isomorphic to a cycle. Thus we choose an edge uv of P_{n-10} of $P_n^{6,6}$ such that $P_n^{6,6} - uv$ contains two components with the same valencies to those of $G - rs$. Note if $G - r - s$ has at least three components, we can obtain a larger graph G' who has just two components by adding some edges to $G - r - s$. We thus have

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G - rs) + b_{2i-2}(G - r - s) \\ &\leqslant b_{2i}(P_n^{6,6} - uv) + b_{2i-2}(P_n^{6,6} - u - v) \\ &= b_{2i}(P_n^{6,6}), \end{aligned}$$

and $G \prec P_n^{6,6}$.

Subcase 1.2.3: $2 \leqslant t \leqslant 5$. If there are some trees planted on both cycles, similar to the proof of Subcase 1.2.2 we can obtain the result. Let $C_a, C_b (a, b \geqslant 6)$ be two cycles of G. Assume that there is no tree planted on C_a. In order to prove the result we first give the following claim:

Claim 2

(i) $P_{b+x}^b \cup P_y \preceq P_{b+x}^6 \cup P_y \preceq P_{n-4}^6 \cup P_4$, *where* $n = b + x + y$ *and* $x \geqslant 1, y \geqslant 4, b \geqslant 8$.
(ii) $P_{n-t}^6 \cup P_t \preceq P_{n-4}^6 \cup P_4$ *for* $n - t \neq 8, n - t \geqslant 7$ *and* $t \geqslant 4$.

Proof. (i) The first inequality is obvious. In the following we will prove the second inequality. It is reduced to prove (ii).

(ii) By Lemma 2 we have

$$b_{2i}(P_{n-t}^{6} \cup P_t) = b_{2i}(P_{n-t} \cup P_t) + b_{2i-2}(P_4 \cup P_t \cup P_{n-t-6}) + 2b_{2i-6}(P_{n-t-6} \cup P_t)$$
$$b_{2i}(P_{n-4}^{6} \cup P_4) = b_{2i}(P_{n-4} \cup P_4) + b_{2i-2}(P_4 \cup P_4 \cup P_{n-10}) + 2b_{2i-6}(P_{n-10} \cup P_4).$$

By Lemma 3 we can obtain the result. □

If $t = 2$, there must be some trees planted on C_b. Let uv be an edge of C_a and u be a vertex of P_t. By Lemma 2 we thus have

$$b_{2i}(G) = b_{2i}(G - uv) + b_{2i-2}(G - u - v) + (-1)^{1+\frac{a}{2}} 2b_{2i-a}(G - C_a)$$
$$b_{2i}(P_n^{6,6}) = b_{2i}(P_n^{6}) + b_{2i-2}(P_{n-6}^{6} \cup P_4) + 2b_{2i-6}(P_{n-6}^{6}).$$

Similar to the above proof, it suffices to prove $b_{2i-2}(G - u - v) \geqslant b_{2i-2}(P_{n-6}^{6} \cup P_4)$.

If $b \geqslant 8$, by Claim 2 the result follows.

If $b = 6$ and $G - u - v \cong P_8^6 \cup P_{n-10}$, then G is the graph obtained from $\Theta(6, n-8, 2)$ by attaching P_3 to C_6. Similar to the above proof we can prove $G \prec \Theta(6, n-8, 4)$.

If $3 \leqslant t \leqslant 5$, let uv be the edge as above. If $G - u - v \ncong P_8^6 \cup P_{n-10}$, similar to above we can obtain the result. If $G - u - v \cong P_8^6 \cup P_{n-10}$, then $G \cong \Theta(6, n-8, 4)$. Deleting the edge of C_6 that is incident to P_4 and applying Lemma 2 we can also obtain the result.

Case 2. $t = 1$. Then G contains two cycles C_a and $C_b (a \geqslant b)$ which have exactly one common vertex w. Let wl be an edge of C_a. Deleting it, we have

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G - wl) + b_{2i-2}(G - w - l) + (-1)^{1+\frac{a}{2}} 2b_{2i-a}(G - C_a) \\ &\leqslant b_{2i}(P_n^{b}) + b_{2i-2}(P_2 \cup P_{n-4}) + 2b_{2i-a}(P_{n-a}) (a \equiv 2 \bmod 4) \\ &\leqslant b_{2i}(P_n^{6}) + b_{2i-2}(P_{n-6}^{6} \cup P_4) + 2b_{2i-6}(P_{n-6}^{6}) \\ &= b_{2i}(P_n^{6,6}), \end{aligned}$$

in which $P_2 \cup P_{n-4} \prec P(n-2; 2, 2) \prec P_{n-4}^{6} \cup P_4$ and the second inequality is proved in Claim 3.

Claim 3. $P(n; 2, 2) \prec P_{n-4}^{6} \cup P_4$.

Proof. It is clear that $b_0(P(n; 2, 2)) = b_0(P_{n-4} \cup P_4) = 1$, $b_2(P(n; 2, 2)) = b_2(P_{n-4} \cup P_4) = n - 1$, $b_4(P(n; 2, 2)) = m(P(n; 2, 2), 2) = n^2 - 5n + 4$ and $b_4(P_{n-4}^{6} \cup P_4) = m(P_{n-4} \cup P_4, 2) = n^2 - 5n + 16$.

In the following we suppose $i \geqslant 3$. By Lemma 2 we have

$$\begin{aligned} b_{2i}(P(n; 2, 2)) &= b_{2i}(P_{n-5} \cup P_5) + b_{2i-2}(P_2 \cup P_2 \cup P_{n-6}) \\ &= b_{2i}(P_{n-5} \cup P_5) + b_{2i-2}(P_2 \cup P_2 \cup P_4 \cup P_{n-10}) \\ &\quad + b_{2i-4}(2P_2 \cup P_3 \cup P_{n-11}) \\ &= b_{2i}(P_{n-5} \cup P_5) + b_{2i-2}(P_2 \cup P_2 \cup P_4 \cup P_{n-10}) \\ &\quad + b_{2i-4}(2P_1 \cup P_2 \cup P_3 \cup P_{n-11}) + b_{2i-6}(P_2 \cup P_3 \cup P_{n-11}) \end{aligned}$$

thus we have

$$\begin{aligned} b_{2i}(P(n;2,2)) &\leqslant b_{2i}(P_{n-4}\cup P_4)+b_{2i-2}(P_2\cup P_2\cup P_4\cup P_{n-10}) \\ &\quad + b_{2i-4}(2P_1\cup P_4\cup P_{n-10})+b_{2i-6}(P_{n-4}\cup P_4) \\ &\leqslant b_{2i}(P_{n-4}\cup P_4)+b_{2i-2}(P_4\cup P_4\cup P_{n-10})+2b_{2i-6}(P_{n-10}\cup P_4) \\ &= b_{2i}(P^6_{n-4}\cup P_4), \end{aligned}$$

we thus complete the proof of Claim 3. □

Combining above all cases we complete the proof. □

Lemma 5. *Let* $G\in\mathscr{B}^2_n(n\geqslant 16)$, *then* $G\prec P^{6,6}_n$.

Proof. Since $G\in\mathscr{B}^2_n$, G also have an center construct which can be viewed as the graph obtained from three paths P_x, P_y and P_z by identifying three pendant vertices (each from one path) into one vertex, and the other three pendant vertices into another vertex. We write it as $\Omega(x,y,z)(x\geqslant y\geqslant z)$. Then G contains three cycles C_{x+y-2}, C_{x+z-2} and C_{y+z-2}.

Case 1. There is no cycle of length 0 (mod 4). Suppose C_a, C_b and C_c are three cycles of G.

Subcase 1.1. The length of longest cycle equals 10. Then G contains one center construct that is isomorphic to one of $\Omega(6,6,2)$, $\Omega(6,6,6)$ and $\Omega(8,4,4)$.

If G contains the center construct $\Omega(6,6,2)$, since $n\geqslant 16$ we can always find an edge uv of C_{10} with vertex u of degree 3 in $\Omega(6,6,2)$ such that $G-u-v$ is not a path, $G-C_6$ is disconnected and is not isomorphic to $P_{n-8}\cup P_2$, where uv is an edge of C_6.

By Lemma 2 we have

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G-uv)+b_{2i-2}(G-u-v)+2b_{2i-10}(G-C_{10})+2b_{2i-6}(G-C_6) \\ b_{2i}(P^{6,6}_n) &= b_{2i}(P^6_n)+b_{2i-2}(P^6_{n-6}\cup P_4)+2b_{2i-6}(P^6_{n-6}). \end{aligned}$$

Clearly, $b_{2i}(G-uv)<b_{2i}(P^6_n)$. By Claim 3 and Lemma 3 we have $b_{2i-2}(G-u-v)\leqslant b_{2i}(P(n-2;2,2))\leqslant b_{2i-2}(P^6_{n-6}\cup P_4)$.

It suffices to prove

$$b_{2i-6}(P^6_{n-6})>b_{2i-10}(G-C_{10})+b_{2i-6}(G-C_6).$$

Since uv is the edge such that $G-C_6\ncong P_2\cup P_{n-8}$, it is easy to prove $G-C_6\preceq P_4\cup P_{n-10}$.

We thus have

$$\begin{aligned} b_{2i-6}(P^6_{n-6}) &\geqslant b_{2i-6}(P_{n-6})+b_{2i-8}(P_4\cup P_{n-12}) \\ &\geqslant b_{2i-6}(P_4\cup P_{n-10})+b_{2i-8}(P_3\cup P_{n-11})+b_{2i-8}(P_4\cup P_{n-12}) \\ &\geqslant b_{2i-6}(P_4\cup P_{n-10})+b_{2i-10}(P_3\cup P_{n-13})+b_{2i-8}(P_4\cup P_{n-12}) \\ &= b_{2i-6}(P_4\cup P_{n-10})+b_{2i-8}(P_{n-8}) \\ &\geqslant b_{2i-6}(P_4\cup P_{n-10})+b_{2i-10}(P_{n-10}) \\ &\geqslant b_{2i-10}(G-C_{10})+b_{2i-6}(G-C_6). \end{aligned}$$

If G contains the center construct $\Omega(6,6,6)$ or $\Omega(8,4,4)$, we choose the edge uv such that u is the vertex of degree 3 in the center construct and contained in two C_{10}'s, say C_{10}^1 and C_{10}^2. Similar to above proof we can prove

$$b_{2i-6}(P_{n-6}^6) > b_{2i-10}(G - C_{10}^1) + b_{2i-10}(G - C_{10}^2).$$

Similarly, we can obtain the result.

Subcase 1.2. There is a cycle of length at least 14.

$$b_{2i-6}(P_{n-6}^6) = b_{2i-6}(P_{n-6}) + b_{2i-8}(P_4 \cup P_{n-12}) \geqslant b_{2i-6}(P_{n-6}) + b_{2i-14}(P_{n-14}).$$

Similar to the proof of Subcase 1.1 we can obtain the result.

Subcase 1.3. The center construct of G is $\Omega(4,4,4)$.

Let B_n be the graph obtained by attaching a pendant vertex of P_{n-7} to a vertex of degree 2 in $\Omega(4,4,4)$ (see Fig. 1).

Claim 4. *If G contains the center construct $\Omega(4,4,4)$, then $G \preceq B_n$ with equality if and only if $G \cong B_n$.*

Proof. We apply induction on n. By simple computation the result is true for $n = 8$ and $n = 9$. We suppose that $n \geqslant 10$ and the result is true for smaller values. Assume that uv is a pendant edge with the pendant vertex v.

If u is a vertex of $\Omega(4,4,4)$, then

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G - v) + b_{2i-2}(G - u - v) \\ &\leqslant b_{2i}(B_{n-1}) + b_{2i-2}(P_{n-2}^6) \\ &\leqslant b_{2i}(B_{n-1}) + b_{2i-2}(B_{n-2}) \\ &= b_{2i}(B_n). \end{aligned}$$

If u is not a vertex of $\Omega(4,4,4)$, then

$$\begin{aligned} b_{2i}(G) &= b_{2i}(G - v) + b_{2i-2}(G - u - v) \\ &\leqslant b_{2i}(B_{n-1}) + b_{2i-2}(B_{n-2}) \\ &= b_{2i}(B_n), \end{aligned}$$

in which we obtain $b_{2i}(G - v) < b_{2i}(B_{n-1})$ by induction hypothesis. Thus we complete the proof of the claim. □

Claim 5. $B_n \prec P_n^{6,6}$.

Proof. By Lemma 2 we have

$$\begin{aligned} b_{2i}(P_n^{6,6}) &= b_{2i}(P_n^6) + b_{2i-2}(P_{n-6}^6 \cup P_4) + 2b_{2i-6}(P_{n-6}^6) \\ &\geqslant b_{2i}(P_n^6) + b_{2i-2}(P_4 \cup P_{n-6}) + b_{2i-4}(2P_4 \cup P_{n-12}) \\ &\quad + 4b_{2i-8}(P_4 \cup P_{n-12}) + 2b_{2i-6}(P_{n-6}) \\ &= b_{2i}(P_n^6) + b_{2i-2}(P_4 \cup P_2 \cup P_{n-8}) + b_{2i-4}(P_4 \cup P_1 \cup P_{n-9}) \\ &\quad + b_{2i-4}(2P_2 \cup P_4 \cup P_{n-12}) + b_{2i-6}(2P_1 \cup P_4 \cup P_{n-12}) \\ &\quad + 4b_{2i-8}(P_4 \cup P_{n-12}) + 2b_{2i-6}(P_{n-6}) \end{aligned}$$

$$
\begin{aligned}
&= b_{2i}(P_n^6) + b_{2i-2}(P_4 \cup P_2 \cup P_{n-8}) + b_{2i-4}(P_4 \cup P_1 \cup P_2 \cup P_{n-11}) \\
&\quad + b_{2i-4}(2P_2 \cup P_4 \cup P_{n-12}) + 2b_{2i-6}(2P_1 \cup P_4 \cup P_{n-11}) \\
&\quad + 4b_{2i-8}(P_4 \cup P_{n-12}) + 2b_{2i-6}(P_{n-6}),
\end{aligned}
$$

and

$$
\begin{aligned}
b_{2i}(B_n) &= b_{2i}(P_n^6) + b_{2i-2}(P(6;2,1) \cup P_{n-8}) + 4b_{2i-6}(P_2 \cup P_{n-8}) \\
&= b_{2i}(P_n^6) + b_{2i-2}(P_4 \cup P_2 \cup P_{n-8}) + b_{2i-4}(2P_1 \cup P_2 \cup P_{n-8}) \\
&\quad + 4b_{2i-6}(P_2 \cup P_{n-8})
\end{aligned}
$$

Since

$$
\begin{aligned}
&2(b_{2i-6}(2P_1 \cup P_4 \cup P_{n-11}) + 2b_{2i-8}(P_4 \cup P_{n-12})) \\
&\quad \geqslant 2(b_{2i-6}(P_2 \cup P_4 \cup P_{n-12}) + b_{2i-8}(P_4 \cup P_{n-11})) \\
&\quad \geqslant 2b_{2i-6}(P_2 \cup P_{n-8})
\end{aligned}
$$

We have $b_{2i}(P_n^{6,6}) \geqslant b_{2i}(B_n)$ and complete the proof of the Claim. □

Case 2. There is a cycle, say C_a, such that $a \equiv 0 \pmod 4$. If $G \ncong \Omega(n-2,3,3)$, we can always find a cycle of length 0 (mod 4), say C_a and an edge uv of it such that u is the vertex of degree 3 of $\Omega(x, y, z)$ and $G - u - v$ is not a path. Deleting it, and applying Lemma 2 we have

$$
\begin{aligned}
&b_{2i}(G) = b_{2i}(G - uv) + b_{2i-2}(G - u - v) - 2b_{2i-a}(G - C_a) + (-1)^{1+\frac{b}{2}} 2b_{2i-b}(G - C_b) \\
&b_{2i}(P_n^{6,6}) = b_{2i}(P_n^6) + b_{2i-2}(P_{n-6}^6 \cup P_4) + 2b_{2i-6}(P_{n-6}^6).
\end{aligned}
$$

Similar to above proof it suffices to prove $G - u - v \prec P_{n-6} \cup P_4$. Since $G - u - v$ is not a path, $G - u - v \preceq P(n-2; 2, 2)$. By Claim 3 we obtain the result.

If $G \cong \Omega(n-2,3,3)$, there are two cycles of lengths $n-1$ in G, since $n \geqslant 16$, similar to the Subcase 1.2 we can also prove the result.

Combining all cases we complete the proof of the lemma. □

By Lemmas 4 and 5 we have

Theorem 1. *Let $G \in \mathscr{B}_n (n \geqslant 16)$. Then $G \preceq P_n^{6,6}$. Moreover, $E(G) \leqslant E(P_n^{6,6})$ with equality if and only if $G \cong P_n^{6,6}$.*

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