MINIMAL ENERGY OF BICYCLIC GRAPHS OF A GIVEN DIAMETER

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Abstract

The energy of a graph is defined as the sum of the absolute values of its eigenvalues. Let $\mathcal{B}(n,d)$ be the class of bicyclic graphs with n vertices, diameter d and containing no vertex-disjoint odd cycles of lengths s and l with $s+l\equiv 2\pmod 4$. In this paper, we characterize the graphs with minimal energy in $\mathcal{B}(n,d)$ for $3\leq d\leq n-3$. We also discuss the case d=n-2.

INTRODUCTION

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

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

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Figure 1: Graph $B_{n,d}$ with $3 \le d \le n - 3$.

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].

A graph whose components are cycles and/or complete graphs with two vertices is called a Sachs graph. Let $\phi(G, \lambda) = \sum_{i=0}^{n} a_i(G) \lambda^{n-i}$. Sachs theorem [1, 2] says that for $i \geq 1$,

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

where L_i denotes the set of Sachs graphs of G with i vertices, p(S) denotes the number of components and c(S) denotes the number of cycles in S. In addition, $a_0(G) = 1$. It is known that E(G) can be expressed as the Coulson integral formula (see [2])

$$E(G) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{dx}{x^2} \log \left[\left(\sum_{i=0}^{\lfloor n/2 \rfloor} (-1)^i a_{2i} x^{2i} \right)^2 + \left(\sum_{i=0}^{\lfloor n/2 \rfloor} (-1)^i a_{2i+1} x^{2i+1} \right)^2 \right], \quad (1)$$

where $a_i = a_i(G)$ for i = 0, 1, ..., n.

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.

From a chemical point of view, it is of greatest interest to find the extremal values of the energy for significant classes of graphs. For instance, Gutman [6] determined the trees with minimal and maximal energies. Hou [7] determined the unicyclic graphs with minimal energy. Yan and Ye [8] determined the trees of a given diameter with minimal energy. Recently, Li and Zhou [9] determined the unicyclic graphs of a given diameter with minimal energy. More results in this direction can be found in Refs. [10–19].

Let $\mathcal{B}(n)$ be the class of bicyclic graphs with n vertices and containing no vertexdisjoint odd cycles of lengths s and l with $s+l\equiv 2\pmod 4$. Let $\mathcal{B}(n,d)$ be the class of bicyclic graphs in $\mathcal{B}(n)$ with diameter d, where $2\leq d\leq n-2$. By a result of Zhang and Zhou [15], for $n\geq 6$, the graph obtained by attaching n-4 pendent vertices to a vertex of degree three of the graph K_4-e (the complete graph on four vertices with one edge deleted) is the unique graph in $\mathcal{B}(n,2)$ with minimal energy. In this paper, we will show that $B_{n,d}$ is the unique graph in $\mathcal{B}(n,d)$ with minimal energy for $3\leq d\leq n-3$, where the graph $B_{n,d}$ is shown in Figure 1. We also discuss the case d=n-2.

PRELIMINARIES

For two graphs G and H, G = H means G and H are isomorphic, and $G \supseteq H$ means G contains a subgraph that is isomorphic to H. For $u \in V(G)$, $\Gamma_G(u)$ denotes the set of neighbors of u in G and the degree of u in G is $\deg_G(u) = |\Gamma_G(u)|$. Let P_n , S_n and C_n be respectively the path, star and cycle on n vertices.

For a graph G with n vertices, let $b_i(G) = |a_i(G)|$ for i = 0, 1, ..., n. Obviously, $b_0(G) = 1$, $b_1(G) = 0$ and $b_2(G)$ equals the number of edges of G. Let $b_i(G) = 0$ if i < 0 or i > n.

Let Q(n) be the class of graphs with n vertices whose components are (i) all trees except at most one being either a unicyclic graph or a bicyclic graph in $\mathcal{B}(m)$ with $4 \leq m \leq n$, or (ii) all trees except two being unicyclic graphs whose union is a subgraph of some graph in $\mathcal{B}(m)$ with $1 \leq m \leq n$.

A quasi-order relation can be introduced in $\mathcal{Q}(n)$: Let $G_1, G_2 \in \mathcal{Q}(n)$. If $b_i(G_1) \geq b_i(G_2)$ for $i = 0, 1, \ldots, n$, then we write $G_1 \succeq G_2$. If $G_1 \succeq G_2$ and there exists a k such that $b_k(G_1) > b_k(G_2)$, then we write $G_1 \succ G_2$.

Note that for any bipartite graph G, $a_{2i+1}(G) = 0$ (see [1, 2]), and that for any $G \in \mathcal{Q}(n)$, $(-1)^i a_{2i}(G) \geq 0$ (see [1, 7, 15]), and moreover, if $G \supseteq K_4 - e$, then $(-1)^i a_{2i+1}(G) \geq 0$ (see [15]). Thus for graphs $G_1, G_2 \in \mathcal{Q}(n)$, if G_2 is bipartite or if $G_1, G_2 \supseteq K_4 - e$, then from (1), we have the following increasing property on E:

$$G_1 \succ G_2 \Rightarrow E(G_1) > E(G_2).$$
 (2)

Lemma 1. Let G be a graph in Q(n).

(a) If uv is a cut edge of G, then

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

(b) Suppose that G contains either a unique cycle C_s or exactly two cycles C_s and C_l and that uv is an edge on C_s . If $s \not\equiv 0 \pmod{4}$, then

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

and if $s \equiv 0 \pmod{4}$, then

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

(c) Suppose that G contains three cycles C_s , C_l and C_r and that uv is a common edge of C_s and C_l . If $s, l \not\equiv 0 \pmod{4}$, then

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

if $s \not\equiv 0 \pmod{4}$ and $l \equiv 0 \pmod{4}$, then

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

and if $s, l \equiv 0 \pmod{4}$, then

$$b_{2i}(G) = b_{2i}(G - uv) + b_{2i-2}(G - u - v) - 2b_{2i-s}(G - C_s) - 2b_{2i-l}(G - C_l).$$

(d) If u is a vertex outside any cycle of G, then

$$b_{2i}(G) = b_{2i}(G-u) + \sum_{u' \in \Gamma_G(u)} b_{2i-2}(G-u-u'),$$

and if G contains three cycles C_s , C_l and C_r and u is a common vertex of them, where $s, l, r \equiv 0 \pmod{4}$, then

$$b_{2i}(G) = b_{2i}(G-u) + \sum_{u' \in \Gamma_G(u)} b_{2i-2}(G-u-u') - 2b_{2i-s}(G-C_s)$$
$$-2b_{2i-l}(G-C_l) - 2b_{2i-r}(G-C_r).$$

Proof. For a graph $G \in \mathcal{Q}(n)$, let $\mathcal{C}(uv)$ and $\mathcal{C}(u)$ denote respectively the sets of all cycles C containing the edge uv and the vertex u in G. Then [1, 2]

$$\phi(G,\lambda) = \phi(G - uv, \lambda) - \phi(G - u - v, \lambda) - 2\sum_{G \in C(uv)} \phi(G - C, \lambda), \tag{3}$$

$$\phi(G,\lambda) = \lambda \phi(G-u,\lambda) - \sum_{u' \in \Gamma_G(u)} \phi(G-u-u',\lambda) - 2 \sum_{C \in \mathcal{C}(u)} \phi(G-C,\lambda). \tag{4}$$

In particular, if uv is a cut edge of G, then

$$\phi(G,\lambda) = \phi(G - uv,\lambda) - \phi(G - u - v,\lambda), \tag{5}$$

and if u is a vertex outside any cycle of G, then

$$\phi(G,\lambda) = \lambda \phi(G-u,\lambda) - \sum_{u' \in \Gamma_G(u)} \phi(G-u-u',\lambda).$$
 (6)

Bearing in mind the facts $(-1)^i a_{2i}(G) \ge 0$ if $G \in \mathcal{Q}(n)$ [1, 7, 15] and $(-1)^i a_{2i+1}(G)$ ≥ 0 (resp. ≤ 0) for $s \equiv 3 \pmod 4$ (resp. $s \equiv 1 \pmod 4$) if G is a unicyclic graph whose unique cycle has length s [7], and equating coefficients of λ^{n-2i} on both sides of identities on characteristic polynomials above, we have (a) from (5), (b) and (c) from (3), and (d) from (6) and (4). \square

By Lemma 1 (a) and Sachs theorem, Lemmas 2 and 3 follow easily.

Lemma 2. Let e be a cut edge of $G \in \mathcal{Q}(n)$. Then $b_{2i}(G) \geq b_{2i}(G-e)$.

Lemma 3. Let G be a unicyclic graph with n vertices or a bicyclic graph in $\mathcal{B}(n)$. Then $G \succ S_n$.

Lemma 4. [2] For $n \ge 2$, $P_n \succeq P_i \cup P_{n-i} \succeq P_1 \cup P_{n-1}$.

Let $\mathcal{T}(n,d)$ be the class of trees with $n \geq 2$ vertices and diameter d, where $1 \leq d \leq n-1$. If $T \in \mathcal{T}(n,1)$, then $T=P_2$. For $1 \leq d \leq n-1$, let $1 \leq T_{n,d}$ denote the graph obtained by attaching $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique tree in $1 \leq t \leq t$ and $1 \leq t \leq t$ are the unique

Lemma 5. [6] For $3 \le d \le n-2$, $P_n \succeq T_{n,d} \succeq S_n$.

Lemma 6. [8] Let $T \in \mathcal{T}(n,d)$ with $3 \le d \le n-2$. Then $T \succeq T_{n,d}$.

Lemma 7. [9] For $3 \le d_0 < d \le n-2$, $T_{n,d} \succeq T_{n,d_0}$.

Lemma 8. For $2 \le d_1 \le n_1 - 2$, we have $T_{n_1,d_1} \cup T \succeq T_{n_1+n_2-1,d_1+d_2}$, where $T = T_{n_2,d_2}$ if $2 \le d_2 \le n_2 - 1$, and P_2 if $n_2 = 2$ and $n_2 = 1$.

Proof. For $2 \le d_2 \le n_2 - 1$, we have $(n_1 - d_1)(n_2 - d_2) \ge n_1 + n_2 - d_1 - d_2 - 1$, and by Lemmas 1 (a) and 4,

$$\begin{split} b_{2i}(T_{n_1,d_1} \cup T_{n_2,d_2}) &= b_{2i}(T_{n_1-1,d_1} \cup T_{n_2,d_2}) + b_{2i-2}(P_{d_1-1} \cup T_{n_2,d_2}) \\ &= b_{2i}(P_{d_1} \cup T_{n_2,d_2}) + (n_1 - d_1)b_{2i-2}(P_{d_1-1} \cup T_{n_2,d_2}) \\ &= b_{2i}(P_{d_1} \cup P_{d_2}) + (n_2 - d_2)b_{2i-2}(P_{d_1} \cup P_{d_2-1}) \\ &\quad + (n_1 - d_1)b_{2i-2}(P_{d_1-1} \cup P_{d_2}) \\ &\quad + (n_1 - d_1)(n_2 - d_2)b_{2i-4}(P_{d_1-1} \cup P_{d_2-1}) \\ &\geq b_{2i}(P_{d_1+d_2-1}) + (n_1 + n_2 - d_1 - d_2)b_{2i-2}(P_{d_1+d_2-2}) \\ &\quad + (n_1 + n_2 - d_1 - d_2 - 1)b_{2i-4}(P_{d_1+d_2-3}) \\ &= b_{2i}(T_{n_1+n_2-1,d_1+d_2}), \end{split}$$

which implies $T_{n_1,d_1} \cup T_{n_2,d_2} \succeq T_{n_1+n_2-1,d_1+d_2}$. It is easy to see that $T_{n_1,d_1} \cup P_2 \succeq T_{n_1+1,d_1+1}$. \Box

Let $\mathcal{U}(n,d)$ be the class of unicyclic graphs with n vertices and diameter d, where $1 \le d \le n-2$. If $U \in \mathcal{U}(n,1)$, then $U = C_3$. For $3 \le d \le n-2$, let $U_{n,d}$ be the graph obtained respectively by attaching n-d-1 pendent vertices and a path P_{d-3} to two non-adjacent vertices of a quadrangle.

Lemma 9. [9] Let $U \in \mathcal{U}(n,d)$ with $3 \leq d \leq n-2$. Then $U \succeq U_{n,d}$.

Lemma 10. For $3 \le d \le n - 2$, $U_{n,d} \succ T_{n,d}$.

Proof. By Lemmas 1 (a) and (b),

$$b_{2i}(U_{n,d}) = b_{2i}(T_{n,d}) + b_{2i-2}(P_{d-3} \cup S_{n-d+1}) - 2b_{2i-4}(P_{d-3})$$

= $b_{2i}(T_{n,d}) + b_{2i-2}(P_{d-3} \cup S_{n-d-1}) \ge b_{2i}(T_{n,d}).$

It is easy to see that $b_2(U_{n,d}) > b_2(T_{n,d})$. Thus $U_{n,d} \succ T_{n,d}$. \square

Lemma 11. For $3 \le d_0 < d \le n - 2$, $U_{n,d} \succeq U_{n,d_0}$.

Proof. If d = 4, then it can be checked that $U_{n,4} \succeq U_{n,3}$ by Sachs theorem. If $d \ge 5$, then by Lemmas 1 (a), 2 and 10,

$$\begin{array}{lcl} b_{2i}(U_{n,d}) & = & b_{2i}(U_{n-1,d-1}) + b_{2i-2}(U_{n-2,d-2}) \\ \\ & \geq & b_{2i}(U_{n-1,d-1}) + b_{2i-2}(T_{n-2,d-2}) \\ \\ & \geq & b_{2i}(U_{n-1,d-1}) + b_{2i-2}(T_{d-1,d-3}) \\ \\ & = & b_{2i}(U_{n,d-1}), \end{array}$$

and so $U_{n,d} \succeq U_{n,d-1} \succeq \cdots \succeq U_{n,d_0}$.

Similarly, we have

Lemma 12. For $3 \le d_0 < d \le n - 3$, $B_{n,d} \succeq B_{n,d_0}$.

MAIN RESULTS

For a graph $G \in \mathcal{B}(n)$, it has either two or three distinct cycles. If G has three cycles, then any two cycles must have at least one edge in common, and we may choose two cycles of lengths of a and b with t common edges such that $a-t \geq t$ and $b-t \geq t$. If G has exactly two cycles, suppose that the lengths of them are a and b respectively. Then, in any case, we choose two cycles C_a and C_b in G. For convenience, let $C_a = v_0v_1 \dots v_{a-1}v_0$ and $C_b = u_0u_1 \dots u_{b-1}u_0$. If C_a and C_b have no common edges, then C_a and C_b are connected by a unique path P, say from v_0 to u_0 . Let l(G) be the length of P. If C_a and C_b have exactly $t \geq 1$ common edges, and thus have exactly $t \geq 1$ common vertices, say, $v_0 = u_0, v_1 = u_1, \dots, v_t = u_t$, then $C_c = u_0u_{b-1} \dots u_{t+1}u_tv_{t+1}v_{t+2} \dots v_{a-1}v_0$ is the third cycle of G, where c = b + a - 2t. If we write $w_0 = u_0, w_1 = u_{b-1}, \dots, w_{c-1} = v_{a-1}$, then $C_c = w_0w_1 \dots w_{c-1}w_0$. Let d(G) be the diameter of G.

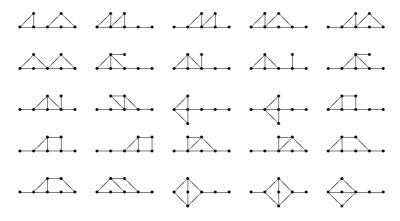


Figure 2: Graphs in $\mathcal{B}(7,4)$ except $B_{7,4}$.

Lemma 13. Let $G \in \mathcal{B}(n, n-3)$ with $n \geq 6$ and $G \neq B_{n,n-3}$. Then $G \succ B_{n,n-3}$.

Proof. We prove this lemma by induction on n.

If n = 6, then by a result of [15] or by direct check, we have $G > B_{6,3}$.

If n = 7, then G is isomorphic to one of the graphs in Figure 2. By Sachs theorem, for $i \ge 3$, we have $b_4(G) > b_4(B_{7,4}) = 7$ and $b_{2i}(B_{7,4}) = 0$. Thus $G > B_{7,4}$.

Suppose that $n \geq 8$ and it is true for all graphs in $\mathcal{B}(n-1, n-4)$ and $\mathcal{B}(n-2, n-5)$. Now suppose that $G \in \mathcal{B}(n, n-3)$ and $G \neq B_{n,n-3}$.

Suppose that there is a pendent vertex u in G such that the degree of its neighbor v is two. Then $G-u\in\mathcal{B}(n-1,n-4)$ and $G-u-v\in\mathcal{B}(n-2,n-5)$. Note that $G\neq B_{n,n-3}$. So $G-u\neq B_{n-1,n-4}$ or $G-u-v\neq B_{n-2,n-5}$. By the induction hypothesis, we have either $G-u\succ B_{n-1,n-4}$ and $G-u-v\succeq B_{n-2,n-5}$ or $G-u\succeq B_{n-1,n-4}$ and $G-u-v\succ B_{n-2,n-5}$. Thus $G\succ B_{n,n-3}$.

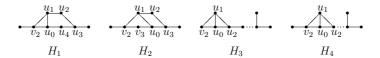


Figure 3: Graphs H_j , $j = 1, \ldots, 4$.

Suppose that the neighbor of any pendent vertex has degree at least three or there is no pendent vertex. Then G is isomorphic to some H_j in Figure 3, j = 1, ..., 4, or G contains one quadrangle which has at most one common vertex with another cycle that is a triangle or a quadrangle. For n = 8, 9, it can be checked by Sachs theorem that $G \succ B_{n,n-3}$. Suppose that $n \ge 10$. Choose C_a and C_b as above. Let $b \ge a$. Note

that $b_4(G) > b_4(B_{n,n-3})$. If $G = H_3$ or H_4 , then and by Lemmas 1 (a), (b) and (c), 2 and 6,

$$b_{2i}(G) = b_{2i}(G - u_0u_2) + b_{2i-2}(G - u_0 - u_2)$$

$$+2b_{2i-3}(G - u_0 - u_1 - u_2) - 2b_{2i-4}(G - u_0 - u_1 - u_2 - v_2)$$

$$\geq b_{2i}(G - u_0u_2 - u_0v_2) + b_{2i-2}(G - u_0 - v_2)$$

$$+b_{2i-2}(G - u_0 - u_2) - 2b_{2i-4}(G - u_0 - u_1 - u_2 - v_2)$$

$$= b_{2i}(G - u_0u_2 - u_0v_2) + b_{2i-2}(G - u_0 - v_2 - u_1u_2)$$

$$+b_{2i-2}(G - u_0 - u_2 - u_1v_2)$$

$$\geq b_{2i}(T_{n,n-3}) + 2b_{2i-2}(P_{n-6}) = b_{2i}(B_{n,n-3}),$$

implying $G \succ B_{n,n-3}$. Otherwise, by Lemmas 1 (a) and (b), 2, 9 and 10,

$$b_{2i}(G) = b_{2i}(G - u_0u_1 - u_1u_2) + b_{2i-2}(G - u_1 - u_2 - u_3u_0)$$

$$+b_{2i-2}(G - u_0 - u_1 - u_2u_3)$$

$$\geq b_{2i}(U_{n-1,n-3}) + b_{2i-2}(U_{n-5,n-7} \cup P_2) + b_{2i-2}(U_{n-4,n-6})$$

$$> b_{2i}(U_{n-1,n-3}) + b_{2i-2}(T_{n-5,n-7} \cup P_2) + b_{2i-2}(T_{n-4,n-6}),$$

while by Lemma 1 (a) and (c),

$$b_{2i}(B_{n,n-3}) = b_{2i}(U_{n-1,n-3}) + b_{2i-2}(P_{n-6} \cup P_2) + b_{2i-2}(P_{n-5}),$$

and so, by Lemma 2, we have $b_{2i}(G) \geq b_{2i}(B_{n,n-3})$ and then $G \succ B_{n,n-3}$.

Lemma 14. Let $G \in \mathcal{B}(n,d)$ with $2 \le d \le n-4$. If G contains no pendent vertices, then $G \succ B_{n,d+1}$.

Proof. We choose C_a , C_b in G and if there exists the third cycle, then we choose C_c and t as above. Let $b \ge a$. Since $d \le n - 4$, we have $b \ge 5$.

Case 1. C_a and C_b have no common edges. Then $d = \lfloor a/2 \rfloor + \lfloor b/2 \rfloor + l(G)$.

Subcase 1.1. $b \not\equiv 0 \pmod{4}$. Then $d(G - u_1 u_2) = \lfloor a/2 \rfloor + b + l(G) - 2 \ge d + 1$, $d(G - u_1 - u_2) \ge d$ and $d \ge 3$. By Lemmas 1 (b), 9, 10 and 11,

$$b_{2i}(G) \geq b_{2i}(G - u_1 u_2) + b_{2i-2}(G - u_1 - u_2)$$

$$\geq b_{2i}(U_{n,d+1}) + b_{2i-2}(U_{n-2,d})$$

$$\geq b_{2i}(U_{n,d+1}) + b_{2i-2}(T_{n-2,d}),$$

and by Lemma 1 (c),

$$b_{2i}(B_{n,d+1}) = b_{2i}(U_{n,d+1}) + b_{2i-2}(P_{d-2} \cup S_{n-d}) - 4b_{2i-4}(P_{d-2}). \tag{7}$$

Hence, by Lemma 2, $b_{2i}(G) \ge b_{2i}(B_{n,d+1})$.

Subcase 1.2. $b \equiv 0 \pmod{4}$. Then $b \geq 8$. Hence $d(G - u_1u_2 - u_2u_3) = \lfloor a/2 \rfloor + b + l(G) - 3 \geq d + 1$, $d(G - u_2 - u_3 - u_4u_5) \geq d - 1$, $d(G - u_1 - u_2 - u_3u_4) \geq d$ and $d \geq 5$. By Lemmas 1 (a) and (b), 9, 10 and 11,

$$b_{2i}(G) = b_{2i}(G - u_1u_2 - u_2u_3) + b_{2i-2}(G - u_2 - u_3)$$

$$+b_{2i-2}(G - u_1 - u_2) - 2b_{2i-b}(G - C_b)$$

$$\geq b_{2i}(G - u_1u_2 - u_2u_3) + b_{2i-2}(G - u_2 - u_3 - u_4u_5)$$

$$+b_{2i-2}(G - u_1 - u_2 - u_3u_4)$$

$$\geq b_{2i}(U_{n-1,d+1}) + b_{2i-2}(U_{n-3,d-1}) + b_{2i-2}(U_{n-3,d})$$

$$\geq b_{2i}(U_{n-1,d+1}) + b_{2i-2}(T_{n-3,d-1}) + b_{2i-2}(T_{n-3,d}),$$

and by Lemma 1 (a) and (c),

$$b_{2i}(B_{n,d+1}) = b_{2i}(U_{n-1,d+1}) + b_{2i-2}(P_{d-2} \cup S_{n-d-2}) + b_{2i-2}(P_{d-1}). \tag{8}$$

Hence, by Lemma 2, $b_{2i}(G) \ge b_{2i}(B_{n,d+1})$.

Case 2. C_a and C_b have at least one common edge. Note that $a-t \ge t$, $b-t \ge t$, where $t \ge 1$. Then $c \ge b$ and $d = \lfloor c/2 \rfloor = \lfloor (a+b)/2 \rfloor - t$.

Subcase 2.1. $b, c \not\equiv 0 \pmod{4}$. Then $d(G - w_0 w_1) = \lfloor a/2 \rfloor + b - t - 1 \ge d + 1$, $d(G - w_0 - w_1) \ge c - 3 \ge d$ and $d \ge 2$. By Lemmas 1 (c), 6, 7, 9 and 11,

$$b_{2i}(G) \ge b_{2i}(G - w_0 w_1) + b_{2i-2}(G - w_0 - w_1) \ge b_{2i}(U_{n,d+1}) + b_{2i-2}(T_{n-2,d}),$$

which, together with (7) and Lemma 2, implies $b_{2i}(G) \ge b_{2i}(B_{n,d+1})$.

Subcase 2.2. $b \not\equiv 0 \pmod{4}$ and $c \equiv 0 \pmod{4}$. If b = 5, then it can be checked by Sachs theorem that $b_{2i}(G) \geq b_{2i}(B_{n,d+1})$. Otherwise, $d(G - w_0w_1 - w_1w_2) = \lfloor a/2 \rfloor + b - t - 2 \geq d + 1$, $d(G - w_1 - w_2 - w_3w_4) \geq d - 1$, $d(G - w_0 - w_1 - w_2w_3) \geq c - 4 \geq d$ and $d \geq 4$. By Lemmas 1 (a), (b) and (c), 6, 7, 9, 10 and 11,

$$\begin{array}{ll} b_{2i}(G) & \geq & b_{2i}(G-w_0w_1-w_1w_2)+b_{2i-2}(G-w_1-w_2-w_3w_4) \\ & & +b_{2i-2}(G-w_0-w_1-w_2w_3) \\ \\ & \geq & b_{2i}(U_{n-1,d+1})+b_{2i-2}(U_{n-3,d-1})+b_{2i-2}(T_{n-3,d}) \\ \\ & > & b_{2i}(U_{n-1,d+1})+b_{2i-2}(T_{n-3,d-1})+b_{2i-2}(T_{n-3,d}), \end{array}$$

which, together with (8) and Lemma 2, implies $b_{2i}(G) \ge b_{2i}(B_{n,d+1})$.

Subcase 2.3. $b \equiv 0 \pmod{4}$ and $c \not\equiv 0 \pmod{4}$. Then $c > b \geq 8$. By similar arguments as those in Subcase 2.2, $b_{2i}(G) \geq b_{2i}(B_{n,d+1})$.

Subcase 2.4. $b, c \equiv 0 \pmod{4}$. Then $a \equiv 0 \pmod{2}$ and $c \geq b \geq 8$. If $a \equiv 2 \pmod{4}$, then $a \geq 6$, and by similar arguments as those in Subcase 2.2, $b_{2i}(G) \geq b_{2i}(B_{n,d+1})$. Suppose that $a \equiv 0 \pmod{4}$. Obviously, n = a + b - t - 1, $d(G - u_0) = c - 2 \geq d + 2$, $d = \lfloor (a+b)/2 \rfloor - t \geq 4$, and $n - 5 \geq d$. By Lemmas 1 (a) and (d), 4, 5, 6 and 7,

$$b_{2i}(G) \geq b_{2i}(G - u_0) + b_{2i-2}(G - u_0 - u_{b-1} - u_t)$$

$$+b_{2i-2}(G - u_0 - u_1 - u_t) + b_{2i-2}(G - u_0 - v_{a-1} - u_t)$$

$$\geq b_{2i}(T_{n-1,d+2}) + b_{2i-2}(P_{a-t-1} \cup P_{b-t-2} \cup P_{t-1})$$

$$+b_{2i-2}(P_{a-t-1} \cup P_{b-t-1} \cup P_{t-2}) + b_{2i-2}(P_{a-t-2} \cup P_{b-t-1} \cup P_{t-1})$$

$$\geq b_{2i}(T_{n-1,d+1}) + 3b_{2i-2}(P_{a+b-t-6})$$

$$\geq b_{2i}(T_{n-1,d+1}) + b_{2i-2}(P_{n-5}) + 2b_{2i-2}(T_{n-5,d-1}),$$

and by Lemma 1 (a), (b) and (c),

$$b_{2i}(B_{n,d+1}) = b_{2i}(T_{n-1,d+1}) + b_{2i-2}(P_d) + 2b_{2i-2}(P_{d-2} \cup S_{n-d-3}). \tag{9}$$

By Lemma 2, $b_{2i}(G) \ge b_{2i}(B_{n,d+1})$.

Combining Cases 1 and 2, we have $b_{2i}(G) \geq b_{2i}(B_{n,d+1})$. Note that $b_4(G) > b_4(B_{n,d+1})$. Thus we have $G \succ B_{n,d+1}$. \square

Lemma 15. Let $G \in \mathcal{B}(n,d)$ with $3 \le d \le n-4$. If G contains exactly one pendent vertex u on all diametrical paths of G such that G-u contains no pendent vertices, then $G \succ B_{n,d+1}$.

Proof. We choose C_a, C_b in G and if there exists the third cycle, then we choose C_c and t as above. Let $b \ge a$. Since $d \le n - 4$, we have $b \ge 5$. Let v be the neighbor of v.

Case 1. C_a and C_b have no common edges. Then $d = \lfloor a/2 \rfloor + \lfloor b/2 \rfloor + l(G) + 1$.

Subcase 1.1. $b \not\equiv 0 \pmod{4}$. If $b \geq 7$, then $d(G - u_1 u_2) \geq \lfloor a/2 \rfloor + b + l(G) - 2 \geq d + 1$. If b = 5, 6, and v lies on C_a , then $d(G - u_1 u_2) = \lfloor a/2 \rfloor + b + l(G) - 1 = d + 1$. If a = 5, b = 6, and v lies on C_b , then $d(G - v_1 v_2) = \lfloor b/2 \rfloor + a + l(G) - 1 = d + 1$. In these cases, by similar arguments as those in Subcase 1.1 of Lemma 14, $b_{2i}(G) \geq b_{2i}(B_{n,d+1})$. Otherwise, a = 3, 4, b = 5, 6, and v lies on C_b . If l(G) = 0, then it can be checked by

Sachs theorem that $b_{2i}(G) \ge b_{2i}(B_{n,d+1})$. Suppose that $l(G) \ge 1$. If a = 3, then by Lemmas 1 (a) and (b), 6 and 9,

$$b_{2i}(G) \geq b_{2i}(G - v_0 v_1) + b_{2i-2}(G - v_0 - v_1 - u_0 u_1)$$

$$\geq b_{2i}(U_{n,d+1}) + b_{2i-2}(T_{n-3,d-1})$$

$$= b_{2i}(U_{n-1,d+1}) + b_{2i-2}(T_{d+1,d-1}) + b_{2i-2}(T_{n-3,d-1}),$$

which, together with (8) and Lemma 2, implies $b_{2i}(G) \ge b_{2i}(B_{n,d+1})$. If a = 4, then n - 4 = d, and by Lemmas 1 (a) and (b), 6 and 8,

$$b_{2i}(G) \geq b_{2i}(G - v_0v_1 - v_1v_2 - u_0u_1) + b_{2i-2}(G - v_0v_1 - v_1v_2 - u_0 - u_1)$$

$$+b_{2i-2}(G - v_0 - v_1 - v_2v_3 - u_0u_1) + b_{2i-2}(G - v_1 - v_2 - v_3v_0 - u_0u_1)$$

$$\geq b_{2i}(T_{n-1,d+1}) + b_{2i-2}(P_{n-b-2} \cup T_{b-1,b-3})$$

$$+b_{2i-2}(T_{n-4,d-2}) + b_{2i-2}(T_{n-3,d-1})$$

$$\geq b_{2i}(T_{n-1,d+1}) + b_{2i-2}(T_{n-4,n-6}) + b_{2i-2}(T_{n-4,d-2}) + b_{2i-2}(T_{n-3,d-1}),$$

which, together with (9) and Lemma 2, implies $b_{2i}(G) \ge b_{2i}(B_{n,d+1})$.

Subcase 1.2. $b \equiv 0 \pmod{4}$. If $b \geq 12$, then $d(G - u_1u_2 - u_2u_3) \geq \lfloor a/2 \rfloor + b + l(G) - 3 \geq d + 2$. If b = 8 and v lies on C_a , then $d(G - u_1u_2 - u_2u_3) = \lfloor a/2 \rfloor + b + l(G) - 2 = d + 1$. In these cases, by similar arguments as those in Subcase 1.2 of Lemma 14, $b_{2i}(G) \geq b_{2i}(B_{n,d+1})$. If a = 5, 6, 7, b = 8, and v lies on C_b , by similar arguments as those in Subcase 1.1 of Lemma 14, $b_{2i}(G) \geq b_{2i}(B_{n,d+1})$. Otherwise, a = 3, 4, b = 8, and v lies on C_b . If $l(G) \leq 2$, then it can be checked by Sachs theorem that $b_{2i}(G) \geq b_{2i}(B_{n,d+1})$. Suppose that $l(G) \geq 3$. By Lemmas 1 (a) and (b), 8, 9 and 10,

$$b_{2i}(G) \geq b_{2i}(G - u_0u_1 - u_1u_2) + b_{2i-2}(G - u_1 - u_2 - u_3u_4)$$

$$+b_{2i-2}(G - u_0 - u_1 - u_2u_3)$$

$$\geq b_{2i}(U_{n-1,d+1}) + b_{2i-2}(U_{n-3,d}) + b_{2i-2}(U_{n-9,d-6} \cup T_{6,4})$$

$$\geq b_{2i}(U_{n-1,d+1}) + b_{2i-2}(T_{n-3,d}) + b_{2i-2}(T_{n-9,d-6} \cup T_{6,4})$$

$$\geq b_{2i}(U_{n-1,d+1}) + b_{2i-2}(T_{n-3,d}) + b_{2i-2}(T_{n-4,d-2}),$$

which, together with (8) and Lemma 2, implies $b_{2i}(G) \ge b_{2i}(B_{n,d+1})$.

Case 2. C_a and C_b have at least one common edge. Then $d = \lfloor c/2 \rfloor + 1 = \lfloor (a+b)/2 \rfloor - t + 1$. Since $b \geq 5$, assume that $w_0, w_1 \neq v$.

If $b, c \not\equiv 0 \pmod{4}$ and $b \ge 6$, then $d(G - w_0 w_1) \ge \lfloor a/2 \rfloor + b - t - 1 \ge d + 1$ and $d(G - w_0 - w_1) \ge c - 3 \ge d - 1$. If $b \not\equiv 0 \pmod{4}$, $c \equiv 0 \pmod{4}$ and $b \ge 9$, then $d(G - w_0 w_1 - w_1 w_2) \ge |a/2| + b - t - 2 \ge d + 1$, $d(G - w_1 - w_2 - w_3 w_4) \ge d - 1$

and $d(G - w_0 - w_1 - w_2w_3) \ge c - 4 \ge d + 1$. If $b \equiv 0 \pmod{4}$ and $c \not\equiv 0 \pmod{4}$, then $d(G - w_0w_1 - w_1w_2) \ge d + 1$, $d(G - w_1 - w_2 - w_3w_4) \ge d - 1$ and $d(G - w_0 - w_1 - w_2w_3) \ge d$. If $a, b, c \equiv 0 \pmod{4}$ and $a \ne 4$ or $b \ne 8$, then $n - d \ge 7$ and $d(G - w_0) \ge c - 2 \ge d + 1$. If $b, c \equiv 0 \pmod{4}$, $a \not\equiv 0 \pmod{4}$ and $a \ge 10$, then $d(G - w_0w_{c-1} - w_{c-1}w_{c-2}) \ge d + 2$, $d(G - w_{c-1} - w_{c-2} - w_{c-3}w_{c-4}) \ge d$ and $d(G - w_0 - w_{c-1} - w_{c-2}w_{c-3}) \ge d + 1$. In these cases, by similar arguments as those in Subcases 2.1-2.4 of Lemma $14, b_{2i}(G) \ge b_{2i}(B_{n,d+1})$.

If $b, c \equiv 0 \pmod{4}$ and a = 6, then $d(G - w_{c-1}w_0 - w_0w_1) \ge c - 2 \ge d + 1$. By Lemmas 1 (a), (b) and (c), 6 and 7,

$$b_{2i}(G) \geq b_{2i}(G - w_{c-1}w_0 - w_0w_1) + b_{2i-2}(G - w_0 - w_1 - w_2w_3)$$

$$+b_{2i-2}(G - w_{c-1} - w_0 - w_1w_2)$$

$$\geq b_{2i}(T_{n,d+1}) + 2b_{2i-2}(T_{n-4,d-1}).$$

By Lemma 1 (b) and (c),

$$b_{2i}(B_{n,d+1}) = b_{2i}(T_{n,d+1}) + 2b_{2i-2}(P_{d-2} \cup S_{n-d-3}). \tag{10}$$

Hence, by Lemma 2, we have $b_{2i}(G) \ge b_{2i}(B_{n,d+1})$.

Now we are left with the cases: (i) $b, c \not\equiv 0 \pmod{4}$ and b = 5, (ii) $b \not\equiv 0 \pmod{4}$, $c \equiv 0 \pmod{4}$ and b = 5, 6, 7, or (iii) $c \equiv 0 \pmod{4}$, a = 4 and b = 8. It can be checked directly by Sachs theorem that $b_{2i}(G) \geq b_{2i}(B_{n,d+1})$.

Combining Cases 1 and 2, we have $b_{2i}(G) \geq b_{2i}(B_{n,d+1})$. Note that $b_4(G) > b_4(B_{n,d+1})$. Thus we have $G \succ B_{n,d+1}$. \square

Theorem 1. Let $G \in \mathcal{B}(n,d)$ with $3 \leq d \leq n-3$. If there are two vertex-disjoint cycles in G, then $G \succ B_{n,d}$.

Proof. We prove this theorem by induction on n-d.

By Lemma 13, the result holds for n - d = 3. Let $h \ge 4$ and suppose that the result holds for n - d < h. Now suppose that n - d = h and $G \in \mathcal{B}(n, d)$.

Case 1. There is no pendent vertex in G. By Lemmas 12 and 14, $G \succ B_{n,d}$.

Case 2. There is a pendent vertex outside some diametrical path $P(G) = x_0x_1 \dots x_d$. Let u, adjacent to v, be a pendent vertex outside P(G) in G. Then $G-u \in \mathcal{B}(n-1,d)$. By the induction hypothesis, $G-u \succ B_{n-1,d}$. By Lemma 1 (a),

$$b_{2i}(B_{n,d}) = b_{2i}(B_{n-1,d}) + b_{2i-2}(T_{d+1,d-2}).$$
(11)

Hence it suffices to show that $b_{2i}(H) \geq b_{2i}(T_{d+1,d-2})$, where H = G - u - v. We choose C_a and C_b in G as above.

Subcase 2.1. v lies on some cycle, say C_a . Then $H \supseteq C_b$.

First, suppose that P(G) and C_b have no common vertices. Then $H \supseteq P_k \cup P_{d-k} \cup C_b$. By Lemmas 2, 3, 4 and 5,

$$b_{2i}(H) \geq b_{2i}(P_k \cup P_{d-k} \cup C_b) \geq b_{2i}(P_{d-1} \cup C_b) \geq b_{2i}(P_{d-1} \cup S_b)$$

$$\geq b_{2i}(P_{d-1} \cup P_3) \geq b_{2i}(P_{d+1}) \geq b_{2i}(T_{d+1,d-2}).$$

Next, suppose that P(G) and C_b have common vertices x_l, \ldots, x_{l+q} , where $q \geq 0$. If v lies outside P(G), then $H \supseteq G_1$, where $G_1 \in \mathcal{U}(s_1, d)$, $s_1 \geq d+2$. By Lemmas 2, 5, 9 and 10,

$$b_{2i}(H) \ge b_{2i}(G_1) \ge b_{2i}(U_{s_1,d}) \ge b_{2i}(T_{s_1,d}) \ge b_{2i}(P_{d+1}) \ge b_{2i}(T_{d+1,d-2}).$$

Suppose that v lies on P(G). Then P(G) and C_a have common vertices, say x_k, \ldots, x_{k+p} , where $p \geq 0$, k+p < l.

If p = 0, then $k \ge 1$, $H \supseteq P_2 \cup P_k \cup G_2$, where $G_2 \in \mathcal{U}(s_2, d_2)$, $s_2 \ge d_2 + 2$, $d_2 \ge d - k - 1 \ge 1$. If $d_2 = 1$, then k = d - 2 and $G_2 = C_3$, and by Lemmas 2, 3, 4 and 5,

$$b_{2i}(H) \ge b_{2i}(P_2 \cup P_{d-2} \cup C_3) \ge b_{2i}(P_{d-1} \cup P_3) \ge b_{2i}(P_{d+1}) \ge b_{2i}(T_{d+1,d-2}).$$

If $d_2 = 2$, then $k \ge d - 3$, $s_2 \ge 4$, and by Lemmas 2, 3, 4, 7 and 8,

$$\begin{array}{ll} b_{2i}(H) & \geq & b_{2i}(P_2 \cup P_k \cup G_2) \geq b_{2i}(P_2 \cup P_k \cup S_{s_2}) \geq b_{2i}(P_2 \cup P_k \cup T_{4,2}) \\ \\ & \geq & b_{2i}(P_{k+1} \cup T_{4,2}) \geq b_{2i}(T_{k+4,k+2}) \geq b_{2i}(T_{d+1,d-1}) \geq b_{2i}(T_{d+1,d-2}). \end{array}$$

If $d_2 \geq 3$, then by Lemmas 2, 4, 7, 8, 9 and 10,

$$b_{2i}(H) \geq b_{2i}(P_2 \cup P_k \cup U_{s_2,d_2}) \geq b_{2i}(P_2 \cup P_k \cup T_{s_2,d_2}) \geq b_{2i}(T_{s_2+k,d_2+k})$$

$$\geq b_{2i}(T_{d_2+k+2,d_2+k}) \geq b_{2i}(T_{d+1,d-1}) \geq b_{2i}(T_{d+1,d-2}).$$

Suppose that p = 1. If $v = x_k$, then $k \ge 1$, $H \supseteq P_k \cup G_3$, where $G_3 \in \mathcal{U}(s_3, d_3)$, $s_3 \ge d_3 + 2$, $d_3 \ge d - k \ge 3$, and by Lemmas 2, 7, 8, 9 and 10,

$$b_{2i}(H) \geq b_{2i}(P_k \cup U_{s_3,d_3}) \geq b_{2i}(P_k \cup T_{s_3,d_3}) \geq b_{2i}(T_{s_3+k-1,d_3+k-1}) \geq b_{2i}(T_{d+1,d-2}).$$

If $v = x_{k+1}$, then $H \supseteq P_{k+2} \cup G_4$, where $G_4 \in \mathcal{U}(s_4, d_4)$, $s_4 \ge d_4 + 2$, $d_4 \ge d - k - 2 \ge 1$. If $d_4 = 1$, then k = d - 3, $G_4 = C_3$, and by Lemmas 2, 3, 4 and 5,

$$b_{2i}(H) \ge b_{2i}(P_{d-1} \cup C_3) \ge b_{2i}(P_{d-1} \cup P_3) \ge b_{2i}(P_{d+1}) \ge b_{2i}(T_{d+1,d-2}).$$

If $d_4 = 2$, then $k \ge d - 4$, $s_4 \ge 4$, and by Lemmas 2, 3, 7 and 8,

$$b_{2i}(H) \ge b_{2i}(P_{k+2} \cup S_{s_4}) \ge b_{2i}(P_{k+2} \cup T_{4,2}) \ge b_{2i}(T_{d+1,d-2}).$$

If $d_4 \geq 3$, then by Lemmas 2, 7, 8, 9 and 10,

$$b_{2i}(H) \ge b_{2i}(P_{k+2} \cup U_{s_4,d_4}) \ge b_{2i}(P_{k+2} \cup T_{s_4,d_4}) \ge b_{2i}(T_{d+1,d-2}).$$

Suppose that $p \geq 2$. If $v \neq x_k, x_{k+p}$, then $H \supseteq G_5$, where $G_5 \in \mathcal{U}(s_5, d), s_5 \geq d+2$. It is easy to show as above that $b_{2i}(H) \geq b_{2i}(T_{d+1,d-2})$. If $v = x_k$, then $k \geq 1$, $H \supseteq P_k \cup G_6$, where $G_6 \in \mathcal{U}(s_6, d_6), s_6 \geq d_6 + 3, d_6 \geq d - k - 1 \geq 3$, and by Lemmas 2, 8, 9 and 10,

$$b_{2i}(H) \ge b_{2i}(P_k \cup U_{s_6,d_6}) \ge b_{2i}(P_k \cup T_{s_6,d_6}) \ge b_{2i}(T_{d+1,d-2}).$$

If $v = x_{k+p}$, then $H \supseteq T_1 \cup G_7$ or $P_{k+p+1} \cup G_7$, where $G_7 \in \mathcal{U}(s_7, d_7)$, $s_7 \ge d_7 + 2$, $d_7 \ge d - k - p - 1 \ge 1$, $T_1 \in \mathcal{T}(k+p+1, k+p-1)$. If $d_7 = 1$, then k+p = d-2, $G_7 = C_3$, and by Lemmas 2, 3, 4, 5, 6, 7 and 8,

$$b_{2i}(H) \ge b_{2i}(T_{d-1,d-3} \cup C_3) \ge b_{2i}(T_{d-1,d-3} \cup P_3) \ge b_{2i}(T_{d+1,d-2}),$$

or

$$b_{2i}(H) \ge b_{2i}(P_{d-1} \cup C_3) \ge b_{2i}(T_{d+1,d-2}).$$

If $d_7 = 2$, then $k + p \ge d - 3$, $s_7 \ge 4$, and by Lemmas 2, 3, 6, 7 and 8,

$$b_{2i}(H) \ge b_{2i}(T_{k+p+1,k+p-1} \cup S_{s_7}) \ge b_{2i}(T_{k+p+1,k+p-1} \cup T_{4,2}) \ge b_{2i}(T_{d+1,d-2}),$$

or

$$b_{2i}(H) \ge b_{2i}(P_{k+p+1} \cup S_{s_7}) \ge b_{2i}(P_{k+p+1} \cup T_{4,2}) \ge b_{2i}(T_{d+1,d-2}).$$

If $d_7 > 3$, then by Lemmas 2, 6, 7, 8, 9 and 10,

$$b_{2i}(H) \ge b_{2i}(T_{k+p+1,k+p-1} \cup U_{s_7,d_7}) \ge b_{2i}(T_{k+p+1,k+p-1} \cup T_{s_7,d_7}) \ge b_{2i}(T_{d+1,d-2}),$$

or

$$b_{2i}(H) \ge b_{2i}(P_{k+p+1} \cup U_{s_7,d_7}) \ge b_{2i}(P_{k+p+1} \cup T_{s_7,d_7}) \ge b_{2i}(T_{d+1,d-2}).$$

Subcase 2.2. v lies outside any cycle. Then $H \supseteq C_a \cup C_b$.

First, suppose that v lies on P(G) and take $v = x_k$. If P(G) and any cycle have no common vertices, then $H \supseteq C_a \cup C_b \cup P_k \cup P_{d-k}$. By Lemmas 2, 3, 4 and 5,

$$b_{2i}(H) \ge b_{2i}(C_a \cup C_b \cup P_k \cup P_{d-k}) \ge b_{2i}(P_3 \cup P_{d-1}) \ge b_{2i}(P_{d+1}) \ge b_{2i}(T_{d+1,d-2}).$$

If P(G) and exactly one cycle, say C_a , have no common vertices, then $H \supseteq C_a \cup P_k \cup G_1$, where $G_1 \in \mathcal{U}(s_1, d_1)$, $s_1 \ge d_1 + 2$, $d_1 \ge d - k - 1 \ge 1$. By Lemmas 2 and 3,

$$b_{2i}(H) \ge b_{2i}(C_a \cup P_k \cup G_1) \ge b_{2i}(P_2 \cup P_k \cup G_1) \ge b_{2i}(T_{d+1,d-2}).$$

If P(G) and both cycles have common vertices, then $H \supseteq P_k \cup G_2$ or $G_3 \cup G_4$, where $G_2 \in \mathcal{B}(s_2, d_2), \ G_3 \in \mathcal{U}(s_3, d_3), \ G_4 \in \mathcal{U}(s_4, d_4), \ d_2 + 3 \le s_2 \le n - 2 - k, d_2 \ge d - k - 1 \ge 2, \ s_3 \ge d_3 + 2, \ d_3 \ge k - 1 \ge 2, \ s_4 \ge d_4 + 2, \ d_4 \ge d - k - 1 \ge 1.$ Suppose that $H \supseteq P_k \cup G_2$. Since $s_2 - d_2 < h$ and $d_2 \ge 4$, by the induction hypothesis, $G_2 \succ B_{s_2,d_2}$. From (10), $b_{2j}(B_{s_2,d_2}) \ge b_{2j}(T_{s_2,d_2})$ for all j. By Lemmas 2 and 8,

$$b_{2i}(H) \ge b_{2i}(P_k \cup G_2) \ge b_{2i}(P_k \cup B_{s_2,d_2}) \ge b_{2i}(P_k \cup T_{s_2,d_2}) \ge b_{2i}(T_{d+1,d-2}).$$

Suppose that $H \supseteq G_3 \cup G_4$. If $d_3 = 2$ and $d_4 = 1$, then d = 5, $s_3 \ge 4$, and by Lemmas 2, 3, 7 and 8,

$$b_{2i}(H) \ge b_{2i}(S_{s_3} \cup C_3) \ge b_{2i}(T_{4,2} \cup P_3) \ge b_{2i}(T_{6,4}) \ge b_{2i}(T_{d+1,d-2}).$$

If $d_3 = 2$, $d_4 = 2$, then $d \le 6$, $s_3 \ge 4$, $s_4 \ge 4$, and by Lemmas 2, 3 and 8,

$$b_{2i}(H) \ge b_{2i}(S_{s_3} \cup S_{s_4}) \ge b_{2i}(T_{4,2} \cup T_{4,2}) \ge b_{2i}(T_{7,4}) \ge b_{2i}(T_{d+1,d-2}).$$

If $d_3 \ge 3$, $d_4 = 1$, then $d_3 \ge d - 3$, and by Lemmas 2, 3, 7, 8, 9 and 10,

$$b_{2i}(H) \ge b_{2i}(U_{s_3,d_3} \cup C_3) \ge b_{2i}(T_{s_3,d_3} \cup P_3) \ge b_{2i}(T_{d+1,d-1}) \ge b_{2i}(T_{d+1,d-2}).$$

If $d_3 \ge 3$, $d_4 = 2$, then $d_3 \ge d - 4$, $s_4 \ge 4$, and by Lemmas 2, 3, 8, 9 and 10,

$$b_{2i}(H) \ge b_{2i}(U_{s_3,d_3} \cup S_{s_4}) \ge b_{2i}(T_{s_3,d_3} \cup T_{4,2}) \ge b_{2i}(T_{d+1,d-2}).$$

If $d_3 \ge 3$, $d_4 \ge 3$, then $d_3 + d_4 \ge d - 2$, and by Lemmas 2, 8, 9 and 10,

$$b_{2i}(H) \ge b_{2i}(U_{s_3,d_3} \cup U_{s_4,d_4}) \ge b_{2i}(T_{s_3,d_3} \cup T_{s_4,d_4}) \ge b_{2i}(T_{d+1,d-2}).$$

Next, suppose that v lies outside P(G). Then $G \supseteq C_a \cup C_b \cup P(G)$, $C_a \cup G_1$ or G_2 , where $G_1 \in \mathcal{U}(s_1, d)$ with $s_1 \ge d + 2$ and $G_2 \in \mathcal{B}(s_2, d)$ with $d + 3 \le s_2 \le n - 2$. It is easy to show as above that $b_{2i}(H) \ge b_{2i}(T_{d+1,d-2})$.

Case 3. Any diametrical path of G contains all pendent vertices. Let $P(G) = x_0x_1...x_d$ be a diametrical path of G. Suppose that $y_0y_1...,y_p$ is a path whose internal vertices $y_1, y_2, ..., y_{p-1}$ all have degree two and y_p is a pendent vertex. Then we say that it is a pendent path, denoted by (y_0, y_p) .

Subcase 3.1. There are exactly two pendent vertices, x_0 and x_d . Suppose that $\deg_G(x_k)$, $\deg_G(x_l) \geq 3$ and that (x_k, x_0) and (x_l, x_d) are distinct pendent paths. Let s = l - k.

Suppose that s=0, i.e. $x_k=x_l$. Then $k\geq 3$ and $l\leq d-3$. Hence it suffices to prove that $G_1,G_2\succ B_{n-d+3,3},\ G_3,G_4\succ S_{n-d+2},$ where $G_1=G-(x_{k-3},x_0)$

 (x_{l+2}, x_d) , $G_3 = G - (x_{k-3}, x_0) - (x_{l+1}, x_d)$, $G_2 = G - (x_{k-2}, x_0) - (x_{l+3}, x_d)$ and $G_4 = G - (x_{k-2}, x_0) - (x_{l+2}, x_d)$. By Lemma 3, $G_3, G_4 \succ S_{n-d+2}$. Let $d_1 = d(G_1)$. Since $d_1 \ge 4$, $n - d + 3 - d_1 < h$. By the induction hypothesis and Lemma 12, $G_1 \succ B_{n-d+3,d_1} \succeq B_{n-d+3,3}$. Similarly, $G_2 \succ B_{n-d+3,3}$.

If s = 1 or 2, then by similar arguments as above, we have the desired result.

Suppose that $s \geq 3$. We need only consider the case $k \geq 2$ and $l \leq d-2$. It suffices to prove that $G_5, G_6 \succ B_{n-d+s+1,s+1}, G_7 \succ B_{n-d+s+2,s+2}$ and $G_8 \succ B_{n-d+s,s}$, where $G_5 = G - (x_{k-2}, x_0) - (x_{l+1}, x_d)$, $G_7 = G - (x_{k-2}, x_0) - (x_{l+2}, x_d)$, $G_8 = G - (x_{k-1}, x_0) - (x_{l+1}, x_d)$ and $G_6 = G - (x_{k-1}, x_0) - (x_{l+2}, x_d)$. Let $d_j = d(G_j)$ and $n_j = |V(G_j)|$, where j = 5, 6, 7, 8. Then $d_j \geq 4$. If $n_j - d_j < h$, then by the induction hypothesis and Lemma 12, we have the desired result.

Suppose that $n_j-d_j=h$. If x_{k-1} lies on all diametrical paths of G_5 , then by Lemmas 12 and 15, $G_5\succ B_{n-d+s+1,s+1}$. Otherwise, by similar arguments as those in Case 2, we also have $G_5\succ B_{n-d+s+1,s+1}$. Similarly, $G_6\succ B_{n-d+s+1,s+1}$. By Lemmas 12 and 14, $G_8\succ B_{n-d+s,s}$. If there exists some diametrical path $P(G_7)$ such that x_{k-1} or x_{l+1} lies outside $P(G_7)$, then by similar arguments as those in Case 2, $G_7\succ B_{n-d+s+2,s+2}$. Otherwise, by Lemmas 1 (a), 2, 9, 10, 11 and 15, $G_7-x_{k-1}\succ B_{n-d+s+1,s+2}, G_7-x_{k-1}-x_k\succeq U_{n-d+s,s}\succ T_{n-d+s,s}\succ T_{s+3,s}$, and then $G_7\succ B_{n-d+s+2,s+2}$.

Subcase 3.2. There is only one pendent vertex. By similar arguments as those in Subcase 3.1, we have the desired result. \Box

Theorem 2. Let $G \in \mathcal{B}(n,d)$ with $3 \leq d \leq n-3$ and $G \neq B_{n,d}$. If there is no vertex-disjoint cycles, then $G \succ B_{n,d}$.

Proof. We prove this theorem by induction on n-d.

By Lemma 13, the result holds for n - d = 3. Let $h \ge 4$ and suppose that the result holds for n - d < h. Now suppose that n - d = h and $G \in \mathcal{B}(n, d)$.

Case 1. There is no pendent vertex in G. By Lemmas 12 and 14, $G \succ B_{n,d}$.

Case 2. There is a pendent vertex outside some diametrical path $P(G) = x_0 x_1 \dots x_d$. Let u, adjacent to v, be a pendent vertex outside P(G). Then $G - u \in \mathcal{B}(n-1,d)$. If $G - u = B_{n-1,d}$, then it can be checked that $G - u - v \succ T_{d+1,d-2}$ (or $T_{4,2}$ if d = 3) and thus from (11), we have $G \succ B_{n,d}$. Otherwise, by the induction hypothesis, $G - u \succ B_{n-1,d}$. So it suffices to show $b_{2i}(H) \ge b_{2i}(T_{d+1,d-2})$ (or $T_{4,2}$ if d = 3), where H = G - u - v. We choose C_a, C_b as above in G and if there exists the third cycle, we denote it by C_c . **Subcase 2.1.** v lies on some cycle, say C_a . Obviously, if $v = u_0$ or u_t , then H contains no cycles. Otherwise, $H \supseteq C_b$ or C_c .

First, suppose that $v = u_0$ or u_t . If v lies outside P(G), then $H \supseteq P(G)$. By Lemmas 2 and 5, $b_{2i}(H) \ge b_{2i}(P_{d+1}) \ge b_{2i}(T_{d+1,d-2})$.

Suppose that v lies on P(G), take $v=x_k$. If C_a and C_b have exactly one common vertex, then $H\supseteq P_2\cup P_2\cup P_k\cup P_{d-k},\ P_2\cup P_k\cup P_{d-k+1},\ P_2\cup P_k\cup T_1,\ P_{k+1}\cup P_{d-k+1},\ P_{k+1}\cup T_1 \text{ or } T_1\cup T_2,\ \text{where } T_1\in \mathcal{T}(d-k+1,d-k-1),\ T_2\in \mathcal{T}(k+1,k-1).$ If C_a and C_b have at least two common vertices, then $H\supseteq P_3\cup P_k\cup P_{d-k},\ P_k\cup P_{d-k+2},\ P_k\cup T_3,\ P_k\cup T_4 \text{ or } P(G),\ \text{where } T_3\in \mathcal{T}(d-k+2,d-k-1),\ T_4\in \mathcal{T}(d-k+2,d-k).$ If $H\supseteq P_2\cup P_2\cup P_k\cup P_{d-k},\ P_2\cup P_k\cup P_{d-k+1},\ P_{k+1}\cup P_{d-k+1},\ P_3\cup P_k\cup P_{d-k},\ P_k\cup P_{d-k+2} \text{ or } P(G),\ \text{then by Lemmas } 2,4\ \text{and } 5,$

$$b_{2i}(H) \ge b_{2i}(P_{d+1}) \ge b_{2i}(T_{d+1,d-2}).$$

If $H \supseteq P_2 \cup P_k \cup T_1$ or $P_{k+1} \cup T_1$, then by Lemmas 2, 4, 6, 7 and 8,

$$b_{2i}(H) \ge b_{2i}(P_{k+1} \cup T_{d-k+1,d-k-1}) \ge b_{2i}(T_{d+1,d-1}) \ge b_{2i}(T_{d+1,d-2}).$$

If $H \supseteq T_1 \cup T_2$, then by Lemmas 2, 6 and 8,

$$b_{2i}(H) \ge b_{2i}(T_{k+1,k-1} \cup T_{d-k+1,d-k-1}) \ge b_{2i}(T_{d+1,d-2}).$$

If $H \supseteq P_k \cup T_3$, then by Lemmas 2, 6 and 8,

$$b_{2i}(H) \ge b_{2i}(P_k \cup T_{d-k+2,d-k-1}) \ge b_{2i}(T_{d+1,d-2}).$$

If $H \supseteq P_k \cup T_4$, the by Lemmas 2, 6, 7 and 8,

$$b_{2i}(H) \ge b_{2i}(P_k \cup T_{d-k+2,d-k}) \ge b_{2i}(T_{d+1,d-1}) \ge b_{2i}(T_{d+1,d-2}).$$

Next, suppose that $v \neq u_0$ and u_t . If v lies outside P(G), then $H \supseteq G_1$ or $P(G) \cup C_s$, where $G_1 \in \mathcal{U}(s_1, d)$, $s_1 \geq d + 2$, s = b or c. If $H \supseteq G_1$, then by Lemmas 2, 5, 9 and 10,

$$b_{2i}(H) \ge b_{2i}(G_1) \ge b_{2i}(U_{s_1,d}) \ge b_{2i}(T_{s_1,d}) \ge b_{2i}(P_{d+1}) \ge b_{2i}(T_{d+1,d-2}).$$

If $H \supseteq P(G) \cup C_s$, then by Lemmas 2, 3 and 5,

$$b_{2i}(H) \ge b_{2i}(P_{d+1} \cup S_s) \ge b_{2i}(P_{d+1}) \ge b_{2i}(T_{d+1,d-2}).$$

Suppose that v lies on P(G). Then P(G) and C_a have vertices, say x_k, \ldots, x_{k+p} , in common, where $p \geq 0$.

If p = 0, then $k \ge 1$, $H \supseteq P_k \cup P_{d-k} \cup C_s$, where s = b or c, and by Lemmas 2, 3, 4 and 5.

$$b_{2i}(H) \ge b_{2i}(P_k \cup P_{d-k} \cup S_s) \ge b_{2i}(P_{d-1} \cup P_3) \ge b_{2i}(P_{d+1}) \ge b_{2i}(T_{d+1,d-2}).$$

Suppose that $p \geq 1$. If $v \neq x_k, x_{k+p}$, then $H \supseteq G_2$, where $G_2 \in \mathcal{U}(s_2,d), s_2 \geq d+2$. It is easy to show as above that $b_{2i}(H) \geq b_{2i}(T_{d+1,d-2})$. Otherwise, for $v = x_k$ or $v = x_{k+p}$, say $v = x_k$, and then $k \geq 1$, $H \supseteq P_k \cup G_3$, $P_k \cup G_4$ or $P_k \cup G'$, where $G_3 \in \mathcal{U}(s_3,d_3), G_4 \in \mathcal{U}(s_4,d_4), s_3 \geq d_3+3, d_3 \geq d-k-1 \geq 2, s_4 \geq d_4+2, d_4 \geq d-k \geq 2$ and G' is the graph obtained by attaching a path P_{d-k-2} to a vertex of $C_b = C_3$. Suppose that $H \supseteq P_k \cup G_3$. If $d_3 = 2$, then k = d-3, $s_3 \geq 5$, and by Lemmas 2, 3 and 8,

$$b_{2i}(H) \ge b_{2i}(P_k \cup S_{s_3}) \ge b_{2i}(P_k \cup T_{5,2}) \ge b_{2i}(T_{d+1,d-2}).$$

If $d_3 \geq 3$, then by Lemmas 2, 8, 9 and 10,

$$b_{2i}(H) \ge b_{2i}(P_k \cup U_{s_3,d_3}) \ge b_{2i}(P_k \cup T_{s_3,d_3}) \ge b_{2i}(T_{d+1,d-2}).$$

Suppose that $H \supseteq P_k \cup G_4$. If $d_4 = 2$, then k = d - 2, $s_4 \ge 4$, and by Lemmas 2, 3, 7 and 8,

$$b_{2i}(H) > b_{2i}(P_k \cup S_{s_4}) > b_{2i}(P_k \cup T_{4,2}) > b_{2i}(T_{d+1,d-1}) > b_{2i}(T_{d+1,d-2}).$$

If $d_4 \geq 3$, then by Lemmas 2, 7, 8, 9 and 10,

$$b_{2i}(H) \ge b_{2i}(P_k \cup U_{s_4,d_4}) \ge b_{2i}(P_k \cup T_{s_4,d_4}) \ge b_{2i}(T_{d+1,d-1}) \ge b_{2i}(T_{d+1,d-2}).$$

Suppose that $H \supseteq P_k \cup G'$. If d-k-2=0, then k=d-2, and by Lemmas 2, 7 and 8,

$$b_{2i}(H) \ge b_{2i}(P_k \cup C_3) \ge b_{2i}(P_k \cup T_{4,2}) \ge b_{2i}(T_{d+1,d-1}) \ge b_{2i}(T_{d+1,d-2}),$$

since it can be checked that $b_{2j}(C_3) \ge b_{2j}(T_{4,2})$. If $d-k-2 \ge 1$, then by Lemmas 1 (a) and (b), 2 and 4,

$$b_{2i}(H) \geq b_{2i}(P_k \cup G' - u_0 u_1) + b_{2i-2}(P_k \cup G' - u_0 - u_1)$$

$$= b_{2i}(P_k \cup T_{d-k+1,d-k-1}) + b_{2i-2}(P_k \cup P_{d-k-1})$$

$$= b_{2i}(P_k \cup P_{d-k-1}) + 2b_{2i-2}(P_k \cup P_{d-k-2}) + b_{2i-2}(P_k \cup P_{d-k-1})$$

$$\geq b_{2i}(P_{d-2}) + 3b_{2i-2}(P_{d-3}) = b_{2i}(T_{d+1,d-2}).$$

Subcase 2.2. v lies outside any cycle. Then H contains two cycles C_a, C_b with at least one common vertex. Let $C_a \cdot C_b$ denote the subgraph of G induced by $V(C_a) \cup V(C_b)$.

First, suppose that v lies on P(G), take $v = x_k$. If vertices on P(G) lie outside any cycle, then $H \supseteq C_a \cdot C_b \cup P_k \cup P_{d-k}$. By Lemmas 2, 3, 4 and 5,

$$b_{2i}(H) \ge b_{2i}(C_a \cdot C_b \cup P_k \cup P_{d-k}) \ge b_{2i}(P_3 \cup P_k \cup P_{d-k}) \ge b_{2i}(T_{d+1,d-2}).$$

If some vertex of P(G) lies on one cycle, then $H \supseteq P_k \cup G_1$, where $G_1 \in \mathcal{B}(s_1, d_1)$, $d_1 + 2 \le s_1 \le n - 2 - k$, $d_1 \ge \max\{d - k - 1, 2\}$. Suppose that $s_1 \ge d_1 + 3$. If $d_1 = 2$, then $k \ge d - 3$, $s_1 \ge 5$, and by Lemmas 2, 3 and 8,

$$b_{2i}(H) \ge b_{2i}(P_k \cup S_{s_1}) \ge b_{2i}(P_k \cup T_{5,2}) \ge b_{2i}(T_{d+1,d-2}).$$

Otherwise, $d_1 \geq 3$, $s_1 - d_1 < h$, and by the induction hypothesis, $G_1 \succeq B_{s_1,d_1}$. Hence by Lemmas 2 and 8 and bearing in mind (10),

$$b_{2i}(H) \ge b_{2i}(P_k \cup G_1) \ge b_{2i}(P_k \cup B_{s_1,d_1}) \ge b_{2i}(P_k \cup T_{s_1,d_1}) \ge b_{2i}(T_{d+1,d-2}).$$

Now suppose that $s_1 = d_1 + 2$. Then G_1 is obtained by attaching respectively paths P_l and P_{d_1-l-2} to the two non-adjacent vertices in $K_4 - e$. If $d_1 = 2$, then $k \ge d - 3$, and by Lemmas 2 and 8,

$$b_{2i}(H) \ge b_{2i}(P_k \cup K_4 - e) \ge b_{2i}(P_k \cup T_{5,2}) \ge b_{2i}(T_{d+1,d-2}),$$

since it can be checked that $b_{2j}(K_4 - e) \ge b_{2j}(T_{5,2})$. If $d_1 \ge 3$, then by Lemmas 1 (a) and (c), 2, 4, 9 and 10,

$$\begin{array}{lcl} b_{2i}(H) & \geq & b_{2i}(P_k \cup G_1 - u_0 u_1) + b_{2i-2}(P_k \cup G_1 - u_0 - u_1) \\ \\ & \geq & b_{2i}(P_k \cup U_{s_1,d_1}) + b_{2i-2}(P_k \cup P_{l+1} \cup P_{d_1-l-1}) \\ \\ & \geq & b_{2i}(P_k \cup T_{d-k+1,d-k-1}) + b_{2i-2}(P_k \cup P_{d-k-2}) \\ \\ & \geq & b_{2i}(T_{d+1,d-2}). \end{array}$$

Next, suppose that v lies outside P(G). Then $G \supseteq C_a \cdot C_b \cup P(G)$ or G_1 , where $G_1 \in \mathcal{B}(s,d)$ with $d+2 \le s \le n-2$. It is easy to show as above that $b_{2i}(H) \ge b_{2i}(T_{d+1,d-2})$.

Case 3. Any diametrical path of G contains all pendent vertices. By similar arguments as those in Case 3 of Theorem 1, $G \succ B_{n,d}$.

Combining Theorems 1 and 2, and using the increasing property (2), we obtain the following main result of this paper.

Theorem 3. Let $G \in \mathcal{B}(n,d)$ with $3 \leq d \leq n-3$ and $G \neq B_{n,d}$. Then $E(G) > E(B_{n,d})$.



Figure 4: Graph B_n^s with $0 \le s \le \lfloor n/2 \rfloor - 2$.

Finally we discuss the case d=n-2. Any graph G in $\mathcal{B}(n,n-2)$ is of the form B_n^s , which is shown in Figure 4, where $0 \le s \le \lfloor n/2 \rfloor - 2$. By direct calculation of the eigenvalues, we find

Conjecture 1. For $n \geq 6$, let

$$s(n) = \begin{cases} 1 & \text{if } n \equiv 1, 3 \pmod{4}, \\ n/2 - 3 & \text{if } n \equiv 2 \pmod{4}, \\ n/2 - 2 & \text{if } n \equiv 0 \pmod{4}. \end{cases}$$

Then for $0 \le s \le \lfloor n/2 \rfloor - 2$ and $s \ne s(n)$, $E(B_n^s) > E(B_n^{s(n)})$.

However, from the the characteristic polynomials, we cannot use the relation " \succ " to deduce $E(B_n^s) > E(B_n^{s(n)})$ for $s \neq s(n)$, as may be seen in Table 1 for $6 \leq n \leq 9$.

Table 1: Characteristic polynomials and energies of B_n^s with $0 \le s \le \lfloor n/2 \rfloor - 2$ and $6 \le n \le 9$.

| | S | coefficients | | | | | | | |
|---|----------|--------------|-------|-------|-------|-------|-------|-------|------------|
| n | | a_3 | a_4 | a_5 | a_6 | a_7 | a_8 | a_9 | $E(B_n^s)$ |
| 6 | 0 = s(6) | -4 | 8 | 6 | 0 | | | | 7.73240 |
| | 1 | -4 | 7 | 4 | -1 | | | | 7.80642 |
| 7 | 0 | -4 | 14 | 10 | -3 | -2 | | | 9.25165 |
| | 1 = s(7) | -4 | 13 | 8 | -4 | -2 | | | 9.21222 |
| | 0 | -4 | 21 | 14 | -11 | -8 | 0 | | 10.32058 |
| 8 | 1 | -4 | 20 | 12 | -11 | -6 | 1 | | 10.37466 |
| | 2 = s(8) | -4 | 20 | 12 | -12 | -8 | 0 | | 10.29253 |
| 9 | 0 | -4 | 29 | 18 | -25 | -18 | 3 | 2 | 11.78220 |
| | 1 = s(9) | -4 | 28 | 16 | -24 | -14 | 5 | 2 | 11.73846 |
| | 2 | -4 | 28 | 16 | -25 | -16 | 4 | 2 | 11.74918 |

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References

- D. Cvetković, M. Doob, H. Sachs, Spectra of Graphs Theory and Application, Johann Ambrosius Barth, Heidelberg, 1995.
- [2] I. Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry, Springer-Verlag, Berlin, 1986.
- [3] I. Gutman, The energy of a graph, Ber. Math.-Statist. Sekt. Forschungszentrum Graz 103 (1978) 1–22.
- [4] I. Gutman, The energy of a graph: Old and new results, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), Algebraic Combinatorics and Applications, Springer-Verlag, Berlin, 2001, pp. 196–211.
- [5] I. Gutman, Topology and stability of conjugated hydrocarbons. The dependence of total π -electron energy on molecular topology, *J. Serb. Chem. Soc.* **70** (2005) 441–456.
- [6] I. Gutman, Acyclic system with extremal Hückel π-electron energy, Theoret. Chim. Acta (Berlin) 45 (1977) 79–87.
- [7] Y. Hou, Unicyclic graphs with minimal energy, J. Math. Chem. 29 (2001) 163– 168.
- [8] W. Yan, L. Ye, On the minimal energy of trees with a given diameter, Appl. Math. Lett. 18 (2005) 1046–1052.
- [9] F. Li, B. Zhou, Minimal energy of unicyclic graphs of a given diameter, *J. Math. Chem.*, in press.
- [10] H. Li, On minimal energy ordering of acyclic conjugated molecules, J. Math. Chem. 29 (1999) 145–169.
- [11] F. Zhang, Z. Li, L. Wang, Hexagonal chains with minimal total π -electron energy, Chem. Phys. Lett. **337** (2001) 125–130.
- [12] F. Li, B. Zhou, Minimal energy of bipartite unicyclic graphs of a given bipartition, MATCH Commun. Math. Comput. Chem. 54 (2005) 379–388.

- [13] Y. Hou, Bicyclic graphs with minimum energy, Lin. Multilin. Algebra 49 (2002) 347–354.
- [14] J. Rada, Energy ordering of catacondensed hexagonal systems, Discr. Appl. Math. 145 (2005) 437–443.
- [15] J. Zhang, B. Zhou, On bicyclic graphs with minimal energies, J. Math. Chem. 37 (2005) 423–431.
- [16] L. Ye, X. Yuan, On the minimal energy of trees with a given number of pendent vertices, MATCH Commun. Math. Comput. Chem. 57 (2007) 193–201.
- [17] H. Hua, On minimal energy of unicyclic graphs with prescribed girth and pendent vertices, MATCH Commun. Math. Comput. Chem. 57 (2007) 351–361.
- [18] H. Hua, Bipartite unicyclic graphs with large energy, MATCH Commun. Math. Comput. Chem. 58 (2007) 57–83.
- [19] I. Gutman, B. Furtula, H. Hua, Bipartite unicyclic graphs with maximal, second-maximal, and third-maximal energy, MATCH Commun. Math. Comput. Chem. 58 (2007) 85–92.