

## On a Conjecture about Tricyclic Graphs with Maximal Energy\*

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### Abstract

For a given simple graph  $G$ , the energy of  $G$ , denoted by  $\mathcal{E}(G)$ , is defined as the sum of the absolute values of all eigenvalues of its adjacency matrix, which was defined by I. Gutman. The problem on determining the maximal energy tends to be complicated for a given class of graphs. There are many approaches on the maximal energy of trees, unicyclic graphs and bicyclic graphs, respectively. Let  $P_n^{6,6,6}$  denote the graph with  $n \geq 20$  vertices obtained from three copies of  $C_6$  and a path  $P_{n-18}$  by adding a single edge between each of two copies of  $C_6$  to one endpoint of the path and a single edge from the third  $C_6$  to the other endpoint of the  $P_{n-18}$ . Very recently, Aouchiche et al. [M. Aouchiche, G. Caporossi, P. Hansen, Open problems on graph eigenvalues studied with AutoGraphiX, *Europ. J. Comput. Optim.* **1**(2013), 181–199] put forward the following conjecture: Let  $G$  be a tricyclic graphs on  $n$  vertices with  $n = 20$  or  $n \geq 22$ , then  $\mathcal{E}(G) \leq \mathcal{E}(P_n^{6,6,6})$  with equality if and only if  $G \cong P_n^{6,6,6}$ . Let  $G(n; a, b, k)$  denote the set of all connected bipartite tricyclic graphs on  $n$  vertices with three vertex-disjoint cycles  $C_a$ ,  $C_b$  and  $C_k$ , where  $n \geq 20$ . In this paper, we try to prove that the conjecture is true for graphs in the class  $G \in G(n; a, b, k)$ , but as a consequence we can only show that this is true for most of the graphs in the class except for 9 families of such graphs.

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## 1 Introduction

Let  $G$  be a graph of order  $n$  and  $A(G)$  be the adjacency matrix of  $G$ . The characteristic polynomial of  $A(G)$  is defined as

$$\phi(G, \lambda) = \det(\lambda I - A(G)) = \sum_{i=0}^n a_i \lambda^{n-i},$$

which is called the *characteristic polynomial* of  $G$ . The  $n$  roots of the equation  $\phi(G, \lambda) = 0$ , denoted by  $\lambda_1, \lambda_2, \dots, \lambda_n$ , are the *eigenvalues* of  $G$ . Since  $A(G)$  is symmetric, all eigenvalues of  $G$  are real. It is well-known [6] that if  $G$  is a bipartite graph, then

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

where  $b_{2i} = (-1)^i a_{2i}$  and  $b_{2i} \geq 0$  for all  $i = 1, \dots, \lfloor \frac{n}{2} \rfloor$ .

The energy of  $G$ , denoted by  $\mathcal{E}(G)$ , is defined as

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

which was proposed by Gutman in 1977 [8]. The following formula is also well-known

$$\mathcal{E}(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log |x^n \phi(G, i/x)| dx,$$

where  $i^2 = -1$ . Moreover, it is known from [6] that the above equality can be expressed as the following explicit formula:

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

where  $a_1, a_2, \dots, a_n$  are the coefficients of  $\phi(G, \lambda)$ . It is also known [11] that for a bipartite graph  $G$ ,  $\mathcal{E}(G)$  can be also expressed as the Coulson integral formula

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

For two bipartite graphs  $G_1$  and  $G_2$ , if  $b_{2i}(G_1) \leq b_{2i}(G_2)$  hold for all  $i = 1, 2, \dots, \lfloor \frac{n}{2} \rfloor$ , we say that  $G_1 \preceq G_2$  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  $G_2 \succ G_1$ . Thus, for two bipartite graphs  $G_1$  and  $G_2$ , we can define the following quasi-order relation,

$$G_1 \preceq G_2 \Rightarrow \mathcal{E}(G_1) \leq \mathcal{E}(G_2), \quad G_1 \prec G_2 \Rightarrow \mathcal{E}(G_1) < \mathcal{E}(G_2).$$

For more results about graph energy, we refer the readers to two surveys [9, 10] and the book [28].

It is quite interesting to study the extremal values of the energy among some given classes of graphs, and characterize the corresponding extremal graphs. In the meantime, a large number of results were obtained on the minimal energies for distinct classes of graphs, such as acyclic conjugated graphs [25, 32], bipartite graphs [30], unicyclic graphs [13, 23], bicyclic graphs [14], tricyclic graphs [26, 27] and tetracyclic graphs [24]. However, the maximal energy problem seems much more difficult than the minimal energy problem. The commonly used comparison method is the so-called quasi-order method. When the graphs are acyclic, bipartite or unicyclic, it is almost always valid. Nevertheless, for general graphs, the quasi-order method is invalid. For these quasi-order incomparable problems, we found an efficient way to determine which one attains the extremal value of the energy, see [16–22].

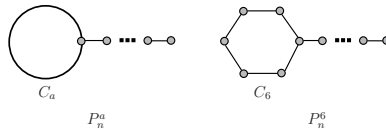


Figure 1.1: Unicyclic graph  $P_n^a$ .

Let  $P_n$ ,  $C_n$  and  $S_n$  be a path, cycle and star graph with  $n$  vertices, respectively. Gutman [8] first considered the extremal values of energy of trees and showed that for any tree  $T$  of order  $n$ ,  $\mathcal{E}(S_n) \leq \mathcal{E}(T) \leq \mathcal{E}(P_n)$ . Let  $P_n^a$  be the graph obtained by connecting a vertex of the cycle  $C_a$  with a terminal vertex of the path  $P_{n-a}$  (as shown in Figure 1.1). In order to find lower and upper bounds of the energy, Caporossi et al. [5] used the AGX system. They proposed a conjecture on the maximal energy of unicyclic graphs.

**Conjecture 1.1** Among all unicyclic graphs on  $n$  vertices, the cycle  $C_n$  has maximal energy if  $n \leq 7$  and  $n = 9, 10, 11, 13$  and  $15$ . For all other values of  $n$ , the unicyclic graph with maximal energy is  $P_n^6$ .

In [15], Hou et al. proved a weaker result, namely that  $\mathcal{E}(P_n^6)$  is maximal within the class of the unicyclic bipartite  $n$ -vertex graphs differing from  $C_n$ . Huo et al. [20] and Andriantiana [1] independently proved that  $\mathcal{E}(C_n) < \mathcal{E}(P_n^6)$ , and then completely determined that  $P_n^6$  is the only graph which attains the maximum value of the energy among all the unicyclic bipartite graphs for  $n = 8, 12, 14$  and  $n \geq 16$ , which partially solves the above conjecture. Finally, Huo et al. [21] and Andriantiana and Wagner [2] completely solved this conjecture by proving the following theorem, independently.

**Theorem 1.2** Among all unicyclic graphs on  $n$  vertices, the cycle  $C_n$  has maximal energy if  $n \leq 7$  but  $n \neq 4$ , and  $n = 9, 10, 11, 13$  and  $15$ ;  $P_4^3$  has maximal energy if  $n = 4$ . For all other values of  $n$ , the unicyclic graph with maximal energy is  $P_n^6$ .

The problem of finding bicyclic graphs with maximum energy was also widely studied. Let  $P_n^{a,b}$  (as shown in Figure 1.2) be the graph obtained from cycles  $C_a$  and  $C_b$  by joining a path of order  $n - a - b + 2$ . Denote by  $R_{a,b}$  the graph obtained from two cycles  $C_a$  and  $C_b$  ( $a, b \geq 10$  and  $a \equiv b \equiv 2 \pmod{4}$ ) by connecting them with an edge. In [12], Gutman and Vidović proposed a conjecture on bicyclic graphs with maximal energy.

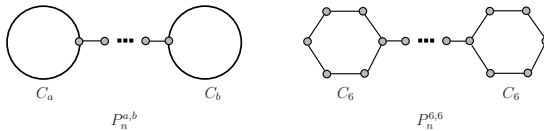


Figure 1.2: Bicyclic graph  $P_n^{a,b}$ .

**Conjecture 1.3** For  $n = 14$  and  $n \geq 16$ , the bicyclic molecular graph of order  $n$  with maximal energy is the molecular graph of the  $\alpha, \beta$  diphenyl-polyene  $C_6H_5(CH)_{n-12}C_6H_5$ , or denoted by  $P_n^{6,6}$ .

Furtula et al. [7] showed by numerical computation that the conjecture is true up to  $n = 50$ . For bipartite bicyclic graphs, Li and Zhang [29] got the following result, giving a partial solution to the above conjecture.

**Theorem 1.4** *If  $G \in \mathcal{B}_n$ , then  $\mathcal{E}(G) \leq \mathcal{E}(P_n^{6,6})$  with equality if and only if  $G \cong P_n^{6,6}$ , where  $\mathcal{B}_n$  denotes the class of all bipartite bicyclic graphs but not the graph  $R_{a,b}$ .*

However, they could not compare the energies of  $P_n^{6,6}$  and  $R_{a,b}$ . Furtula et al. in [7] showed by numerical computation that  $\mathcal{E}(P_n^{6,6}) > \mathcal{E}(R_{a,b})$ , which implies that the conjecture is true for bipartite bicyclic graphs. They only performed the computation up to  $a + b = 50$ . It is evident that a solid mathematical proof is still needed. Huo et al. [19] completely solved this problem. However, the conjecture is still open for non-bipartite bicyclic graphs.

**Theorem 1.5** *Let  $G$  be any connected, bipartite bicyclic graph with  $n$  ( $n \geq 12$ ) vertices. Then  $\mathcal{E}(G) \leq \mathcal{E}(P_n^{6,6})$  with equality if and only if  $G \cong P_n^{6,6}$ .*

Actually, Wagner [31] showed that the maximum value of the graph energy within the set of all graphs with cyclomatic number  $k$  (which includes, for instance, trees or unicyclic graphs as special cases) is at most  $4n/\pi + c_k$  for some constant  $c_k$  that only depends on  $k$ . However, the corresponding extremal graphs are not considered.

The problem of finding the tricyclic graphs maximizing the energy remains open. Gutman and Vidović [12] listed some tricyclic molecular graphs that might have maximal energy for  $n \leq 20$ . Very recently, in [3], experiments using AutoGraphiX led us to conjecture the structure of tricyclic graphs that presumably maximize energy for  $n = 6, \dots, 21$ . For  $n \geq 22$ , Aouchiche et al. [3] proposed a general conjecture obtained with AutoGraphiX. First, let  $P_n^{6,6,6}$  (as shown in Figure 1.3) denote the graph on  $n \geq 20$  obtained from three copies of  $C_6$  and a path  $P_{n-18}$  by adding a single edge between each of two copies of  $C_6$  to one endpoint of the path and a single edge from the third  $C_6$  to the other endpoint of the  $P_{n-18}$ .

**Conjecture 1.6** *Let  $G$  be a tricyclic graphs on  $n$  vertices with  $n = 20$  or  $n \geq 22$ . Then  $\mathcal{E}(G) \leq \mathcal{E}(P_n^{6,6,6})$  with equality if and only if  $G \cong P_n^{6,6,6}$ .*

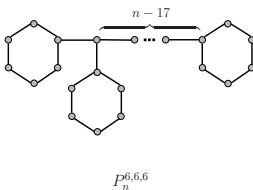


Figure 1.3: Tricyclic graph  $P_n^{6,6,6}$ .

Let  $G(n; a, b, k)$  denote the set of all connected bipartite tricyclic graphs on  $n$  vertices with three disjoint cycles  $C_a$ ,  $C_b$  and  $C_k$ , where  $n \geq 20$ . In this paper, we try to prove that the conjecture is true for graphs in the class  $G \in G(n; a, b, k)$ , but as a consequence we can only show that this is true for most of the graphs in the class except for 9 families of such graphs.

## 2 Preliminaries

The following are the elementary results on the characteristic polynomial of graphs and graph energy, which will be used in our proof.

**Lemma 2.1** [6] *Let  $uv$  be an edge of  $G$ . Then*

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

where  $\varphi(uv)$  is the set of cycles containing  $uv$ . In particular, if  $uv$  is a pendant edge of  $G$  with the pendant vertex  $v$ , then

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

**Lemma 2.2** *Let  $uv$  be an edge of a bipartite tricyclic graph  $G$  which contains three vertex-disjoint cycles. Then*

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

where  $\varphi(uv)$  is the set of cycles containing  $uv$ . In particular, if  $uv$  is a pendant edge of  $G$  with the pendant vertex  $v$ , then

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

*Proof.* By Lemma 2.1, we have

$$a_{2i}(G) = a_{2i}(G - uv) - a_{2i-2}(G - u - v) - 2 \sum_{C_1 \in \varphi(uv)} a_{2i-1}(G - C_1)$$

and

$$\begin{aligned} (-1)^i a_{2i}(G) &= (-1)^i a_{2i}(G - uv) + (-1)^{i-1} a_{2i-2}(G - u - v) \\ &\quad + 2 \sum_{C_1 \in \varphi(uv)} (-1)^{1+\frac{1}{2}} (-1)^{i-\frac{1}{2}} a_{2i-1}(G - C_1). \end{aligned}$$

Since  $b_{2i} = (-1)^i a_{2i}$ , then the result follows. ■

From Sachs Theorem [6], we can obtain the following properties for bipartite graphs.

**Proposition 2.3** (1). *If  $G_1$  and  $G_2$  are both 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  $G$  and  $G + e$  both be 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  $2 \pmod{4}$  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  $b_{2i}(G_0) \geq 0$  and  $b_{2i}(G_1) \geq b_{2i}(G_2)$  for all positive integer  $i$ , we have  $G_0 \cup G_1 \preceq G_0 \cup G_2$ . Moreover, for bipartite graphs  $G_i, G'_i, i = 1, 2$ , if  $G_i$  has the same order as  $G'_i$  and  $G_i \preceq G'_i$ , then  $G_1 \cup G_2 \preceq G'_1 \cup G'_2$ .*

**Lemma 2.4** [11] *Let  $n = 4k, 4k + 1, 4k + 2$  or  $4k + 3$ . Then*

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

From the definition of  $G(n; a, b, k)$ , we know that  $a, b$  and  $k$  are all even. We will divide  $G(n; a, b, k)$  into two categories  $G_I(n; a, b, k; l_1, l_2; l_c)$  and  $G_{II}(n; a, b, k; l_1, l_2, l_3)$  in the following.

We say that  $H$  is the *central structure* of  $G$  if  $G$  can be viewed as the graph obtained from  $H$  by planting some trees on it. The central structures of  $G_I(n; a, b, k; l_1, l_2; l_c)$  and  $G_{II}(n; a, b, k; l_1, l_2, l_3)$  are  $\Theta_I(n; a, b, k; l_1, l_2; l_c)$  and  $\Theta_{II}(n; a, b, k; l_1, l_2, l_3)$ , respectively.

$\Theta_I(n; a, b, k; l_1, l_2; l_c)$  (as shown in Figure 2.4) is the set of all the elements of  $G(n; a, b, k)$  in which  $C_a$  and  $C_b$  are joined by a path  $P_1 = u_1 \cdots u_2$  ( $u_2 \in V(C_b)$ ) with  $l_1$  vertices,  $C_k$  and  $C_b$  are joined by a path  $P_2 = v_1 \cdots v_2$  ( $v_2 \in V(C_b)$ ) with  $l_2$  vertices. In addition, the smaller part  $u_2 \cdots v_2$  of  $C_b$  has  $l_c$  vertices. Note that when  $u_2 = v_2$ , we have  $l_c = 1$ .

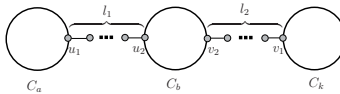


Figure 2.4:  $\Theta_I(n; a, b, k; l_1, l_2; l_c)$ .

$\Theta_{II}(n; a, b, k; l_1, l_2, l_3)$  (as shown in Figure 2.5) is also a subset of  $G(n; a, b, k)$ . For any  $G \in \Theta_{II}(n; a, b, k; l_1, l_2, l_3)$ ,  $G$  has a center vertex  $v$ ,  $C_a, C_b$  and  $C_k$  are joined to  $v$  by paths  $P_1 = u_1 \cdots v$  ( $u_1 \in V(C_a)$ ),  $P_2 = u_2 \cdots v$  ( $u_2 \in V(C_b)$ ),  $P_3 = u_3 \cdots v$  ( $u_3 \in V(C_k)$ ), respectively. The number of vertices of  $P_1, P_2$  and  $P_3$  are  $l_1, l_2$  and  $l_3$ , respectively.

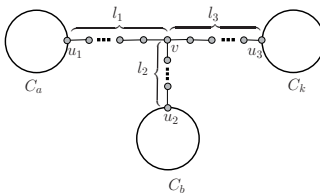


Figure 2.5:  $\Theta_{II}(n; a, b, k; l_1, l_2, l_3)$ .



It is easy to verify that

$$G(n; a, b, k) = G_I(n; a, b, k; l_1, l_2; l_c) \cup G_{II}(n; a, b, k; l'_1, l'_2, l'_3).$$

Now we define two special graph classes  $\Gamma_1$  and  $\Gamma_2$  as follows.

$\Gamma_1$  consists of graphs  $G$  with the following four different possible forms:

- (i)  $G \in \Theta_I(n; a, 4, k; l_1, l_2; 2)$ , where  $a \geq 8, k \geq 8, 2 \leq l_1 \leq 3, 2 \leq l_2 \leq 3$ .
- (ii)  $G \in \Theta_I(n; a, b, k; l_1, l_2; 2)$ , where  $a \geq 8, b \geq 6, k \geq 8, 2 \leq l_1 \leq 3, 2 \leq l_2 \leq 3$  and  $l_1 = l_2 = 3$  is not allowed.
- (iii)  $G \in \Theta_I(n; 4, b, k; l_1, l_2; 2)$ , where  $b \geq 6, k \geq 6, 2 \leq l_1 \leq 3$  and  $2 \leq l_2 \leq 3$ .
- (iv)  $G \in \Theta_I(n; a, b, 4; l_1, l_2; 2)$ , where  $2 \leq l_2 \leq 3$ .

Whereas  $\Gamma_2$  consists of graphs  $G$  with the following five different possible forms:

- (i)  $G \in \Theta_{II}(n; a, b, k; 2, l_2, l_3)$ , where  $a \geq 8$ .
- (ii)  $G \in \Theta_{II}(n; a, b, k; 3, 3, 3)$ , where  $a \geq k \geq b \geq 8$ .
- (iii)  $G \in \Theta_{II}(n; a, 4, k; l_1, 3, l_3)$ .
- (iv)  $G \in \Theta_{II}(n; a, 4, k; l_1, 2, l_3)$ .
- (v)  $G \in \Theta_{II}(n; a, 4, k; 3, 4, 3)$ , where  $a \geq k \geq 6$ .

In this paper, we first try to find the graphs with maximal energy among the two categories of  $G(n; a, b, k)$ :  $G_I(n; a, b, k; l_1, l_2; l_c)$  and  $G_{II}(n; a, b, k; l_1, l_2, l_3)$ , respectively. Then, we will obtain that  $P_n^{6,6,6} = \Theta_{II}(n; 6, 6, 6; n - 17, 2, 2)$  has the maximal energy among all graphs in  $G(n; a, b, k)$  except for two classes  $\Gamma_1$  and  $\Gamma_2$ . Our main result is stated as follows, which gives support to Conjecture 1.6.

**Theorem 2.5** *For any tricyclic bipartite graph  $G \in G(n; a, b, k) \setminus (\Gamma_1 \cup \Gamma_2)$ ,  $\mathcal{E}(G) \leq \mathcal{E}(P_n^{6,6,6})$  and the equality holds if and only if  $G \cong P_n^{6,6,6}$ .*

### 3 Proof of Theorem 2.5.

By repeatedly applying the recursive formula of  $b_{2i}(G)$  in Lemma 2.2 and the third property in Proposition 2.3, we obtain the following two lemmas.

**Lemma 3.1** *If  $G \in G_I(n; a, b, k; l_1, l_2; l_c) \setminus \Theta_I(n; a, b, k; l'_1, l'_2; l'_c)$ , then there exists a graph  $G' \in \Theta_I(n; a, b, k; l'_1, l'_2; l'_c)$  such that  $G \prec G'$ , i.e., the graph with maximal energy among graphs in  $G_I(n; a, b, k; l_1, l_2; l_c)$  must belong to  $\Theta_I(n; a, b, k; l'_1, l'_2; l'_c)$ .*

**Lemma 3.2** *If  $G \in G_{II}(n; a, b, k; l_1, l_2, l_3) \setminus \Theta_{II}(n; a, b, k; l'_1, l'_2, l'_3)$ , then there exists a graph  $G' \in \Theta_{II}(n; a, b, k; l'_1, l'_2, l'_3)$  such that  $G \prec G'$ , i.e., the graph with maximal energy among graphs in  $G_{II}(n; a, b, k; l_1, l_2, l_3)$  must belong to  $\Theta_{II}(n; a, b, k; l'_1, l'_2, l'_3)$ .*

From the results above, we know that the graph with maximal energy among graphs in  $G(n; a, b, k)$  must belong to  $\Theta_I(n; a, b, k; l_1, l_2; l_c)$  or  $\Theta_{II}(n; a, b, k; l_1, l_2, l_3)$ . Therefore, in the following, we will find the graph with maximal energy among graphs in  $\Theta_I(n; a, b, k; l_1, l_2; l_c)$  and  $\Theta_{II}(n; a, b, k; l_1, l_2, l_3)$ .

**Lemma 3.3** *For any graph  $G \in \Theta_I(n; a, b, k; l_1, l_2; l_c)$ , there exists a graph  $H \in \Theta_I(n; a, b, k; l_1, l_2; 2)$  such that  $G \preceq H$ .*

*Proof.* We distinguish the following two cases:

**Case 1.**  $l_c = 1$ .

For fixed parameters  $n, a, b, k, l_1$  and  $l_2$ , let  $G_1 \in \Theta_I(n; a, b, k; l_1, l_2; 1)$  and  $G_2 = \Theta_I(n; a, b, k; l_1, l_2; 2)$  (as shown in Figure 3.6). It suffices to show that  $G_1 \preceq G_2$ .

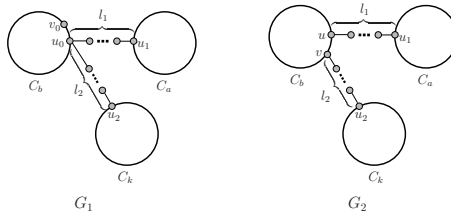


Figure 3.6: Graphs for Lemma 3.3.

By Lemma 2.2 we have

$$b_{2i}(G_1) = b_{2i}(G_1 - u_0v_0) + b_{2i-2}(G_1 - u_0 - v_0) + (-1)^{1+\frac{i}{2}} 2b_{2i-b}(G_1 - C_b)$$

$$\begin{aligned}
 &= b_{2i}(G_1 - u_0v_0) + b_{2i-2}(P_{a+l_1-2}^a \cup P_{k+l_2-2}^k \cup P_{b-2}) \\
 &\quad + (-1)^{1+\frac{b}{2}} 2b_{2i-b}(P_{a+l_1-2}^a \cup P_{k+l_2-2}^k)
 \end{aligned}$$

and

$$\begin{aligned}
 b_{2i}(G_2) &= b_{2i}(G_2 - uv) + b_{2i-2}(G_2 - u - v) + (-1)^{1+\frac{b}{2}} 2b_{2i-b}(G_2 - C_b) \\
 &= b_{2i}(G_2 - uv) + b_{2i-2}(P_{a+l_1-2}^a \cup P_{k+l_2-2}^k \cup P_{b-2}) \\
 &\quad + (-1)^{1+\frac{b}{2}} 2b_{2i-b}(P_{a+l_1-2}^a \cup P_{k+l_2-2}^k).
 \end{aligned}$$

Therefore, it suffices to show that  $b_{2i}(G_1 - u_0v_0) \leq b_{2i}(G_2 - uv)$ . By Lemma 2.2 we have

$$\begin{aligned}
 b_{2i}(G_1 - u_0v_0) &= b_{2i}(P_{a+l_1-2}^a \cup P_{k+b+l_2-2}^k) + b_{2i-2}(P_{a+l_1-3}^a \cup P_{k+l_2-2}^k \cup P_{b-1}) \\
 b_{2i}(G_2 - uv) &= b_{2i}(P_{a+l_1-2}^a \cup P_{k+b+l_2-2}^k) + b_{2i-2}(P_{a+l_1-3}^a \cup P_{k+b+l_2-3}^k) \\
 &= b_{2i}(P_{a+l_1-2}^a \cup P_{k+b+l_2-2}^k) + b_{2i-2}(P_{a+l_1-3}^a \cup P_{k+l_2-2}^k \cup P_{b-1}) \\
 &\quad + b_{2i-4}(P_{a+l_1-3}^a \cup P_{k+l_2-3}^k \cup P_{b-2}).
 \end{aligned}$$

Since  $b_{2i-4}(P_{a+l_1-3}^a \cup P_{k+l_2-3}^k \cup P_{b-2}) \geq 0$ , then we obtain  $b_{2i}(G_1 - u_0v_0) \leq b_{2i}(G_2 - uv)$ .

**Case 2.**  $l_c \geq 2$ .

For fixed parameters  $n, a, b, k, l_1$  and  $l_2$ , let  $G'_1 \in \Theta_I(n; a, b, k; l_1, l_2; l_c)$  and  $G'_2 \in \Theta_I(n; a, b, k; l_1, l_2; 2)$  (as shown in Figure 3.7, where  $u_3$  belongs to the part of  $C_b$  with length  $b - l_c + 1$ ). It suffices to show that  $G'_1 \preceq G'_2$ .

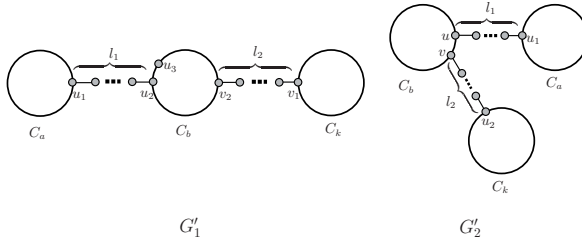


Figure 3.7: Graphs for Lemma 3.3.

By Lemma 2.2 we have

$$b_{2i}(G'_1) = b_{2i}(G'_1 - u_2u_3) + b_{2i-2}(G'_1 - u_2 - u_3) + (-1)^{1+\frac{b}{2}} 2b_{2i-b}(G'_1 - C_b);$$

$$b_{2i}(G'_2) = b_{2i}(G'_2 - uv) + b_{2i-2}(G'_2 - u - v) + (-1)^{1+\frac{k}{2}} 2b_{2i-b}(G'_2 - C_b).$$

Since  $(-1)^{1+\frac{k}{2}} 2b_{2i-b}(G'_1 - C_b) = (-1)^{1+\frac{k}{2}} 2b_{2i-b}(G'_2 - C_b)$ , we only need to compare  $b_{2i}(G'_1 - u_2u_3) + b_{2i-2}(G'_1 - u_2 - u_3)$  with  $b_{2i}(G'_2 - uv) + b_{2i-2}(G'_2 - u - v)$ . By applying Lemma 2.2 repeatedly, we have

$$\begin{aligned} & b_{2i}(G'_1 - u_2u_3) + b_{2i-2}(G'_1 - u_2 - u_3) \\ = & b_{2i}(P_{a+l_1+l_c-3}^a \cup P_{b+k+l_2-l_c-1}^k) + b_{2i-2}(P_{a+l_1+l_c-4}^a \cup P_{k+l_2-2}^k \cup P_{b-l_c}) \\ & + b_{2i-2}(P_{a+l_1-2}^a \cup P_{k+l_2-2}^k \cup P_{b-2}) + b_{2i-4}(P_{a+l_1-2}^a \cup P_{k+l_2-3}^k \cup P_{l_c-2} \cup P_{b-l_c-1}), \end{aligned}$$

and

$$\begin{aligned} & b_{2i}(G'_2 - uv) + b_{2i-2}(G'_2 - u - v) \\ = & b_{2i}(P_{a+l_1+l_c-3}^a \cup P_{b+k+l_2-l_c-1}^k) + b_{2i-2}(P_{a+l_1+l_c-4}^a \cup P_{k+l_2-2}^k \cup P_{b-l_c}) \\ & + b_{2i-2}(P_{a+l_1-2}^a \cup P_{k+l_2-2}^k \cup P_{b-2}) \\ = & b_{2i}(P_{a+l_1+l_c-3}^a \cup P_{b+k+l_2-l_c-1}^k) + b_{2i-2}(P_{a+l_1+l_c-4}^a \cup P_{k+l_2-2}^k \cup P_{b-l_c}) \\ & + b_{2i-4}(P_{a+l_1+l_c-4}^a \cup P_{k+l_2-3}^k \cup P_{b-l_c-1}) + b_{2i-2}(P_{a+l_1-2}^a \cup P_{k+l_2-2}^k \cup P_{b-2}) \\ = & b_{2i}(P_{a+l_1+l_c-3}^a \cup P_{b+k+l_2-l_c-1}^k) + b_{2i-2}(P_{a+l_1+l_c-4}^a \cup P_{k+l_2-2}^k \cup P_{b-l_c}) \\ & + b_{2i-2}(P_{a+l_1-2}^a \cup P_{k+l_2-2}^k \cup P_{b-2}) + b_{2i-4}(P_{a+l_1-2}^a \cup P_{k+l_2-3}^k \cup P_{l_c-2} \cup P_{b-l_c-1}) \\ & + b_{2i-6}(P_{a+l_1-3}^a \cup P_{k+l_2-3}^k \cup P_{l_c-3} \cup P_{b-l_c-1}). \end{aligned}$$

Since  $b_{2i-6}(P_{a+l_1-3}^a \cup P_{k+l_2-3}^k \cup P_{l_c-3} \cup P_{b-l_c-1}) \geq 0$ , we have  $b_{2i}(G'_1 - u_2u_3) + b_{2i-2}(G'_1 - u_2 - u_3) \leq b_{2i}(G'_2 - uv) + b_{2i-2}(G'_2 - u - v)$ .

Thus, the proof is complete. ■

**Theorem 3.4** *For any graph  $G \in \Theta_{II}(n; a, b, k; l_1, l_2, l_3) \setminus \Gamma_2$ , there exists a graph  $H \in \Theta_{II}(n; 6, 6, 6; l'_1, l'_2, l'_3)$  such that  $G \preceq H$ .*

*Proof.* Without loss of generality, we may assume that  $a \geq k \geq b$ . It is obvious that  $l_1, l_2, l_3 \geq 2$ . We distinguish the following cases:

$$\text{Case 1. } \begin{cases} l_1 + a - 2 \geq 7 \\ l_2 + b - 3 \geq 7 \\ l_3 + k - 2 \geq 7 \end{cases}$$

In this case, considering the values of  $l_1$ ,  $l_2$  and  $l_3$ , we distinguish the following four subcases.

**Subcase 1.1.**  $l_1 \geq 3$ ,  $l_2 \geq 4$  and  $l_3 \geq 3$ .

For any values of  $l_1$ ,  $l_2$  and  $l_3$ , let  $G_1 \in \Theta_{II}(n; a, b, k; l_1, l_2, l_3)$  and  $G_{01} \in \Theta_{II}(n; 6, 6, 6; l'_1, l'_2, l'_3)$  (as shown in Figure 3.8), where  $l'_1 = a + l_1 - 6$ ,  $l'_2 = b + l_2 - 6$  and  $l'_3 = k + l_3 - 6$ .

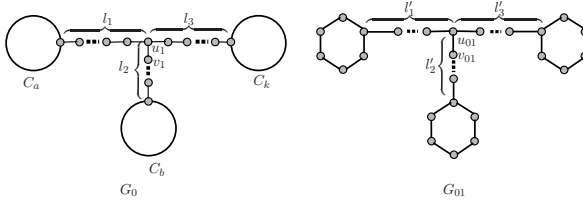


Figure 3.8: Graphs for Subcase 1.1.

By Lemma 2.2, we have

$$\begin{aligned}
 b_{2i}(G_1) &= b_{2i}(G_1 - u_1 v_1) + b_{2i-2}(G_1 - u_1 - v_1) \\
 &= b_{2i}(P_{a+k+l_1+l_3-3}^a \cup P_{b+l_2-2}^b) + b_{2i-2}(P_{a+l_1-2}^a \cup P_{k+l_3-2}^k \cup P_{b+l_2-3}^b), \\
 b_{2i}(G_{01}) &= b_{2i}(G_{01} - u_{01} v_{01}) + b_{2i-2}(G_{01} - u_{01} - v_{01}) \\
 &= b_{2i}(P_{l'_1+l'_3+9}^{6,6} \cup P_{l'_2+4}^6) + b_{2i-2}(P_{l'_1+4}^6 \cup P_{l'_3+4}^6 \cup P_{l'_2+3}^6) \\
 &= b_{2i}(P_{a+k+l_1+l_3-3}^{6,6} \cup P_{b+l_2-2}^6) + b_{2i-2}(P_{a+l_1-2}^6 \cup P_{k+l_3-2}^6 \cup P_{b+l_2-3}^6).
 \end{aligned}$$

By Proposition 2.3, we can obtain that  $G_1 \leq G_{01}$ .

**Subcase 1.2.**  $l_1 = 2$ ,  $l_2 \geq 4$ ,  $l_3 \geq 3$  or  $l_1 \geq 3$ ,  $l_2 \geq 4$ ,  $l_3 = 2$ .

The graphs in this subcase belong to  $\Gamma_2(i)$ , so we do not consider them.

**Subcase 1.3.**  $l_1 \geq 3$ ,  $l_2 = 3$ ,  $l_3 \geq 3$ .

It is easy to verify that  $b \geq 8$  and then we have  $a \geq k \geq b \geq 8$ . Let  $G_2 \in \Theta_{II}(n; a, b, k; l_1, l_2, l_3)$  and  $G_{02} \in \Theta_{II}(n; 6, 6, 6; l'_1, l'_2, l'_3)$ , where  $l'_1 = a + l_1 - 6$ ,  $l'_2 = b + l_2 - 6$  and  $l'_3 = k + l_3 - 6$ . If  $l_1 > 3$  or  $l_3 > 3$ , then with similar analysis in Subcase 1.1, we have

$$b_{2i}(G_2) = b_{2i}(P_{k+b+l_2+l_3-3}^{k,b} \cup P_{a+l_1-2}^a) + b_{2i-2}(P_{a+l_1-3}^a \cup P_{k+l_3-2}^k \cup P_{b+l_2-2}^b),$$

$$\begin{aligned} b_{2i}(G_{02}) &= b_{2i}(P_{l'_2+l'_3+9}^{6,6} \cup P_{l'_1+4}^6) + b_{2i-2}(P_{l'_1+3}^6 \cup P_{l'_3+4}^6 \cup P_{l'_2+4}^6) \\ &= b_{2i}(P_{k+b+l_2+l_3-3}^{6,6} \cup P_{a+l_1-2}^6) + b_{2i-2}(P_{a+l_1-3}^6 \cup P_{k+l_3-2}^6 \cup P_{b+l_2-2}^6). \end{aligned}$$

By Proposition 2.3, we can obtain that  $G_2 \preceq G_{02}$ .

If  $l_1 = l_2 = l_3 = 3$ , the graphs in this case belong to  $\Gamma_2(ii)$ , so we do not consider them.

**Subcase 1.4.**  $l_1 \geq 3$ ,  $l_2 = 2$ ,  $l_3 \geq 3$  or  $l_1 = l_3 = 2$ ,  $l_2 \geq 4$  or  $l_1 = 2$ ,  $2 \leq l_2 \leq 3$ ,  $l_3 \geq 3$  or  $l_1 \geq 3$ ,  $2 \leq l_2 \leq 3$ ,  $l_3 = 2$  or  $l_1 = l_3 = 2$ ,  $2 \leq l_2 \leq 3$ .

The graphs in this case belong to  $\Gamma_2(i)$ , so we do not consider them.

$$\text{Case 2. } \begin{cases} l_1 + a - 2 \leq 6 \\ l_2 + b - 3 \geq 7 \\ l_3 + k - 2 \geq 7 \end{cases}$$

In this case, it is easy to verify that  $a \leq 6$ , from which we have  $b \leq k \leq a \leq 6$ . If  $a = b = k = 6$ , it follows that this lemma holds. Hence, we consider the following subcases.

**Subcase 2.1.**  $a = k = 6$ ,  $b = 4$ .

It is easy to verify that  $l_2 \geq 6$  and  $l_3 \geq 3$ . For any values of  $l_2$  and  $l_3$ , let  $G_3 \in \Theta_{II}(n; 6, 4, 6; 2, l_2, l_3)$  and  $G_{03} \in \Theta_{II}(n; 6, 6, 6; 2, l'_2, l'_3)$ , where  $l'_2 = l_2 - 2$  and  $l'_3 = l_3$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_3) &= b_{2i}(P_{l_3+11}^{6,6} \cup P_{l_2+2}^4) + b_{2i-2}(C_6 \cup P_{l_3+4}^6 \cup P_{l_2+1}^4), \\ b_{2i}(G_{03}) &= b_{2i}(P_{l_3+11}^{6,6} \cup P_{l_2+2}^6) + b_{2i-2}(C_6 \cup P_{l_3+4}^6 \cup P_{l_2+1}^6). \end{aligned}$$

By Proposition 2.3, we can obtain that  $G_3 \preceq G_{03}$ .

**Subcase 2.2.**  $a = 6$ ,  $k = b = 4$ .

It is easy to verify that  $l_2 \geq 6$  and  $l_3 \geq 5$ . For any values of  $l_2$  and  $l_3$ , let  $G_3 \in \Theta_{II}(n; 6, 4, 4; 2, l_2, l_3)$  and  $G_{03} \in \Theta_{II}(n; 6, 6, 6; 2, l'_2, l'_3)$ , where  $l'_2 = l_2 - 2$  and  $l'_3 = l_3 - 2$ . By Lemma 2.2, we have

$$b_{2i}(G_4) = b_{2i}(P_{l_3+9}^{6,4} \cup P_{l_2+2}^4) + b_{2i-2}(C_6 \cup P_{l_3+2}^4 \cup P_{l_2+1}^4),$$

$$b_{2i}(G_{04}) = b_{2i}(P_{l_3+9}^{6,6} \cup P_{l_2+2}^6) + b_{2i-2}(C_6 \cup P_{l_3+2}^6 \cup P_{l_2+1}^6).$$

By Proposition 2.3, we can obtain that  $G_4 \preceq G_{04}$ .

**Subcase 2.3.**  $a = k = b = 4$ .

It is easy to verify that  $l_1 \leq 4$ ,  $l_2 \geq 6$  and  $l_3 \geq 5$ . If  $l_1 = 4$ , let  $G_5 \in \Theta_{II}(n; 4, 4, 4; 4, l_2, l_3)$  and  $G_{05} \in \Theta_{II}(n; 6, 6, 6; 2, l'_2, l'_3)$ , where  $l'_2 = l_2 - 2$  and  $l'_3 = l_3 - 2$ . By Lemma 2.2, we have

$$b_{2i}(G_5) = b_{2i}(P_{l_3+9}^{4,4} \cup P_{l_2+2}^4) + b_{2i-2}(P_6^4 \cup P_{l_3+2}^4 \cup P_{l_2+1}^4),$$

$$b_{2i}(G_{05}) = b_{2i}(P_{l_3+9}^{6,6} \cup P_{l_2+2}^6) + b_{2i-2}(C_6 \cup P_{l_3+2}^6 \cup P_{l_2+1}^6).$$

Also,  $\phi(P_6^4; \lambda) = \lambda^6 - 6\lambda^4 + 6\lambda^2$  and  $\phi(C_6; \lambda) = \lambda^6 - 6\lambda^4 + 9\lambda^2 - 4$ . It follows that  $P_6^4 \prec C_6$ . By Proposition 2.3, we can obtain that  $G_5 \preceq G_{05}$ .

If  $l_1 < 4$ , graphs in this case belong to  $\Gamma_2(iii)$  or  $\Gamma_2(iv)$ , so we do not consider them.

$$\text{Case 3. } \begin{cases} l_1 + a - 2 \geq 7 \\ l_2 + b - 3 \geq 7 \\ l_3 + k - 2 \leq 6 \end{cases}$$

In this case, it is easy to verify that  $k \leq 6$ . If  $b \leq k \leq a \leq 6$ , with similar analysis in Case 2 we obtain that this lemma holds. Then we consider the case  $a > 6 \geq k \geq b$ . Without considering graphs with forms  $\Gamma_2(i)$ ,  $\Gamma_2(iii)$  and  $\Gamma_2(iv)$ , there are only two subclasses as follows.

**Subcase 3.1.**  $a > 6$ ,  $k = 6$ ,  $b = 6$  or  $4$ .

It is easy to verify that  $l_2 \geq 4$  and  $l_3 = 2$ . We have  $l_1 \geq 3$  since we do not consider graphs with form  $\Gamma_2(i)$ . For any values of  $l_1$  and  $l_3$ , let  $G_6 \in \Theta_{II}(n; a, b, 6; l_1, l_2, 2)$  and  $G_{06} \in \Theta_{II}(n; 6, 6, 6; l'_1, l'_2, 2)$ , where  $l'_1 = a + l_1 - 6$  and  $l'_2 = b + l_2 - 6$ . By Lemma 2.2, we have

$$b_{2i}(G_6) = b_{2i}(P_{a+l_1+5}^{a,6} \cup P_{b+l_2-2}^b) + b_{2i-2}(P_{a+l_1-2}^a \cup C_6 \cup P_{b+l_2-3}^b),$$

$$b_{2i}(G_{06}) = b_{2i}(P_{a+l_1+5}^{6,6} \cup P_{b+l_2-2}^6) + b_{2i-2}(P_{a+l_1-2}^6 \cup C_6 \cup P_{b+l_2-3}^6).$$

By Proposition 2.3, we can obtain that  $G_6 \preceq G_{06}$ .

**Subcase 3.2.**  $a > 6$ ,  $k = b = 4$ .

It is easy to verify that  $l_2 \geq 6$  and  $l_3 \leq 4$ . We have  $l_1 \geq 3$  since we do not consider graphs with form  $\Gamma_2(i)$ . For any values of  $l_1$  and  $l_3$ , let  $G_7 \in \Theta_{II}(n; a, 4, 4; l_1, l_2, 4)$  and  $G_{07} \in \Theta_{II}(n; 6, 6, 6; l'_1, l'_2, 2)$ , where  $l'_1 = a + l_1 - 6$  and  $l'_2 = l_2 - 2$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_7) &= b_{2i}(P_{a+l_1+5}^{a,4} \cup P_{l_2+2}^4) + b_{2i-2}(P_{a+l_1-2}^a \cup P_6^4 \cup P_{l_2+1}^4), \\ b_{2i}(G_{07}) &= b_{2i}(P_{a+l_1+5}^{6,6} \cup P_{l_2+2}^6) + b_{2i-2}(P_{a+l_1-2}^6 \cup C_6 \cup P_{l_2+1}^6). \end{aligned}$$

Also,  $P_6^4 \prec C_6$ . By Proposition 2.3, we can obtain that  $G_7 \preceq G_{07}$ .

$$\text{Case 4. } \begin{cases} l_1 + a - 2 \geq 7 \\ l_2 + b - 3 \leq 6 \\ l_3 + k - 2 \geq 7 \end{cases}$$

It is easy to verify that  $b \leq 6$ . Without considering graphs with forms  $\Gamma_2(i)$ ,  $\Gamma_2(iii)$ ,  $\Gamma_2(iv)$  and  $\Gamma_2(v)$ , we can distinguish this case into the following four subcases.

**Subcase 4.1.**  $b = 6$ ,  $l_2 = 3$ ,  $l_1 \geq 3$  and  $l_3 \geq 3$ .

For any values of  $l_1$  and  $l_3$ , let  $G_8 \in \Theta_{II}(n; a, 6, k; l_1, 3, l_3)$  and  $G_{08} \in \Theta_{II}(n; 6, 6, 6; l'_1, 3, l'_3)$ , where  $l'_1 = a + l_1 - 6$  and  $l'_3 = k + l_3 - 6$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_8) &= b_{2i}(P_{a+k+l_1+l_3-3}^{a,k} \cup P_7^6) + b_{2i-2}(P_{a+l_1-2}^a \cup P_{k+l_3-2}^k \cup C_6), \\ b_{2i}(G_{08}) &= b_{2i}(P_{a+k+l_1+l_3-3}^{6,6} \cup P_7^6) + b_{2i-2}(P_{a+l_1-2}^6 \cup P_{k+l_3-2}^6 \cup C_6). \end{aligned}$$

By Proposition 2.3, we can obtain that  $G_8 \preceq G_{08}$ .

**Subcase 4.2.**  $b = 6$ ,  $l_3 = 2$ ,  $l_1 \geq 3$  and  $l_3 \geq 3$ .

For any values of  $l_1$  and  $l_3$ , let  $G_9 \in \Theta_{II}(n; a, 6, k; l_1, 2, l_3)$  and  $G_{09} \in \Theta_{II}(n; 6, 6, 6; l'_1, 2, l'_3)$ , where  $l'_1 = a + l_1 - 6$  and  $l'_3 = k + l_3 - 6$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_9) &= b_{2i}(P_{a+k+l_1+l_3-3}^{a,k} \cup C_6) + b_{2i-2}(P_{a+l_1-2}^a \cup P_{k+l_3-2}^k \cup P_5), \\ b_{2i}(G_{09}) &= b_{2i}(P_{a+k+l_1+l_3-3}^{6,6} \cup C_6) + b_{2i-2}(P_{a+l_1-2}^6 \cup P_{k+l_3-2}^6 \cup P_5). \end{aligned}$$

By Proposition 2.3, we have  $G_9 \preceq G_{09}$ .

**Subcase 4.3.**  $b = 4$ ,  $l_3 = 5$ ,  $l_1 \geq 3$  and  $l_3 \geq 3$ .



For any values of  $l_1$  and  $l_3$ , let  $G_{10} \in \Theta_{II}(n; a, 4, k; l_1, 5, l_3)$  and  $G_{010} \in \Theta_{II}(n; 6, 6, 6; l'_1, 3, l'_3)$ , where  $l'_1 = a + l_1 - 6$  and  $l'_3 = k + l_3 - 6$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{10}) &= b_{2i}(P_{a+k+l_1+l_3-3}^{a,k} \cup P_7^4) + b_{2i-2}(P_{a+l_1-2}^a \cup P_{k+l_3-2}^k \cup P_6^4), \\ b_{2i}(G_{010}) &= b_{2i}(P_{a+k+l_1+l_3-3}^{6,6} \cup P_7^6) + b_{2i-2}(P_{a+l_1-2}^6 \cup P_{k+l_3-2}^6 \cup C_6). \end{aligned}$$

By Proposition 2.3, we can obtain that  $G_{10} \preceq G_{010}$ .

**Subcase 4.4.**  $b = 4, l_2 = 4, l_1 \geq 3$  and  $l_3 \geq 3$ .

Let  $G_{11} \in \Theta_{II}(n; a, 4, k; l_1, 4, l_3)$  and  $G_{011} \in \Theta_{II}(n; 6, 6, 6; l'_1, 2, l'_3)$ , where  $l'_1 = a + l_1 - 6$  and  $l'_3 = k + l_3 - 6$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{11}) &= b_{2i}(P_{a+k+l_1+l_3-3}^{a,k} \cup P_6^4) + b_{2i-2}(P_{a+l_1-2}^a \cup P_{k+l_3-2}^k \cup P_5^4), \\ b_{2i}(G_{011}) &= b_{2i}(P_{a+k+l_1+l_3-3}^{6,6} \cup C_6) + b_{2i-2}(P_{a+l_1-2}^6 \cup P_{k+l_3-2}^6 \cup P_5). \end{aligned}$$

Also,  $\phi(P_5^4; \lambda) = \lambda^5 - 3\lambda^3 + 2\lambda$  and  $\phi(P_5; \lambda) = \lambda^5 - 4\lambda^3 + 3\lambda$ . So  $P_5^4 \prec P_5$ . Then by Proposition 2.3, we have  $G_{11} \preceq G_{011}$ .

$$\text{Case 5. } \begin{cases} l_1 + a - 2 \leq 6 \\ l_2 + b - 3 \geq 7 \\ l_3 + k - 2 \leq 6 \end{cases}$$

It is easy to verify that  $a \leq 6$  and then we have  $b \leq k \leq a \leq 6$ . If  $a = b = k = 6$ , it follows that this lemma holds. Then we focus on other subcases. Without considering graphs with forms  $\Gamma_2(iii), \Gamma_2(iv)$ , we can distinguish this case into the following three subcases.

**Subcase 5.1.**  $a = k = 6, b = 4$ .

It is easy to verify that  $l_1 = l_3 = 2$  and  $l_2 \geq 6$ . For any value of  $l_2$ , let  $G_{12} \in \Theta_{II}(n; 6, 4, 6; 2, l_2, 2)$  and  $G_{012} \in \Theta_{II}(n; 6, 6, 6; 2, l'_2, 2)$ , where  $l'_2 = l_2 - 2$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{12}) &= b_{2i}(P_{13}^{6,6} \cup P_{l_2+2}^4) + b_{2i-2}(C_6 \cup C_6 \cup P_{l_2+1}^4), \\ b_{2i}(G_{012}) &= b_{2i}(P_{13}^{6,6} \cup P_{l_2+2}^6) + b_{2i-2}(C_6 \cup C_6 \cup P_{l_2+1}^6). \end{aligned}$$

By Proposition 2.3, we can obtain that  $G_{12} \preceq G_{012}$ .

**Subcase 5.2.**  $a = 6, k = b = 4, l_3 = 4.$

It is easy to verify that  $l_1 = 2.$  For fixed  $l_2,$  let  $G_{13} \in \Theta_{II}(n; 6, 4, 4; 2, l_2, 4)$  and  $G_{013} \in \Theta_{II}(n; 6, 6, 6; 2, l_2', 4),$  where  $l_2' = l_2 - 2.$  By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{13}) &= b_{2i}(P_{l_2+9}^{4,4} \cup C_6) + b_{2i-2}(P_5 \cup P_6^4 \cup P_{l_2+2}^4), \\ b_{2i}(G_{013}) &= b_{2i}(P_{l_2+9}^{6,6} \cup C_6) + b_{2i-2}(P_5 \cup C_6 \cup P_{l_2+2}^6). \end{aligned}$$

By Proposition 2.3, we have  $G_{13} \preceq G_{013}.$

**Subcase 5.3.**  $a = k = b = 4, l_1 = l_3 = 4.$

It is easy to verify that  $l_2 \geq 6.$  For fixed  $l_2,$  let  $G_{14} \in \Theta_{II}(n; 4, 4, 4; 4, l_2, 4)$  and  $G_{014} \in \Theta_{II}(n; 6, 6, 6; 2, l_2', 2),$  where  $l_2' = l_2 - 2.$  By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{14}) &= b_{2i}(P_{13}^{4,4} \cup P_{l_2+2}^4) + b_{2i-2}(P_6^4 \cup P_6^4 \cup P_{l_2+1}^4), \\ b_{2i}(G_{014}) &= b_{2i}(P_{13}^{6,6} \cup P_{l_2+2}^6) + b_{2i-2}(C_6 \cup C_6 \cup P_{l_2+1}^6). \end{aligned}$$

Also,  $P_6^4 \prec C_6,$  and by Proposition 2.3, we can obtain that  $G_{14} \preceq G_{014}.$

$$\text{Case 6. } \begin{cases} l_1 + a - 2 \leq 6 \\ l_2 + b - 3 \leq 6 \\ l_3 + k - 2 \geq 7 \end{cases}$$

It is easy to verify that  $a \leq 6$  and then we have  $b \leq k \leq a \leq 6.$  If  $a = b = k = 6,$  it follows that this lemma holds. Then we focus on other subcases. Without considering graphs with forms  $\Gamma_2(iii), \Gamma_2(iv),$  we can distinguish this case into the following three subcases.

**Subcase 6.1.**  $a = k = 6, b = 4, 4 \leq l_2 \leq 5.$

It is easy to verify that  $l_1 = 2, l_3 \geq 3.$  For any values of  $l_2$  and  $l_3,$  let  $G_{15} \in \Theta_{II}(n; 6, 4, 6; 2, l_2, l_3)$  and  $G_{015} \in \Theta_{II}(n; 6, 6, 6; 2, l_2', l_3'),$  where  $l_2' = l_2 - 2, l_3' = l_3.$  By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{15}) &= b_{2i}(P_{l_2+9}^{6,4} \cup P_{l_3+4}^6) + b_{2i-2}(C_6 \cup P_{l_2+2}^4 \cup P_{l_3+3}^6), \\ b_{2i}(G_{015}) &= b_{2i}(P_{l_2+9}^{6,6} \cup P_{l_3+4}^6) + b_{2i-2}(C_6 \cup P_{l_2+2}^6 \cup P_{l_3+3}^6). \end{aligned}$$

By Proposition 2.3, we can obtain that  $G_{15} \preceq G_{015}.$

**Subcase 6.2.**  $a = 6, k = b = 4, 4 \leq l_2 \leq 5$ .

It is easy to verify that  $l_1 = 2, l_3 \geq 5$ . For any values of  $l_2$  and  $l_3$ , let  $G_{16} \in \Theta_{II}(n; 6, 4, 4; 2, l_2, l_3)$  and  $G_{016} \in \Theta_{II}(n; 6, 6, 6; 2, l'_2, l'_3)$ , where  $l'_2 = l_2 - 2, l'_3 = l_3 - 2$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{16}) &= b_{2i}(P_{l_2+9}^{6,4} \cup P_{l_3+2}^4) + b_{2i-2}(C_6 \cup P_{l_2+2}^4 \cup P_{l_3+1}^4), \\ b_{2i}(G_{016}) &= b_{2i}(P_{l_2+9}^{6,6} \cup P_{l_3+2}^6) + b_{2i-2}(C_6 \cup P_{l_2+2}^6 \cup P_{l_3+1}^6). \end{aligned}$$

By Proposition 2.3, we can obtain that  $G_{16} \preceq G_{016}$ .

**Subcase 6.3.**  $a = k = b = 4, l_1 = 4, 4 \leq l_2 \leq 5$ .

It is easy to verify that  $l_3 \geq 5$ . For any values of  $l_2$  and  $l_3$ , let  $G_{17} \in \Theta_{II}(n; 4, 4, 4; 4, l_2, l_3)$  and  $G_{017} \in \Theta_{II}(n; 6, 6, 6; 2, l'_2, l'_3)$ , where  $l'_2 = l_2 - 2, l'_3 = l_3 - 2$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{17}) &= b_{2i}(P_{l_2+9}^{4,4} \cup P_{l_3+2}^4) + b_{2i-2}(P_6^4 \cup P_{l_2+2}^4 \cup P_{l_3+1}^4), \\ b_{2i}(G_{017}) &= b_{2i}(P_{l_2+9}^{6,6} \cup P_{l_3+2}^6) + b_{2i-2}(C_6 \cup P_{l_2+2}^6 \cup P_{l_3+1}^6). \end{aligned}$$

Also,  $P_6^4 \prec C_6$ , and by Proposition 2.3, we have  $G_{17} \preceq G_{017}$ .

$$\text{Case 7. } \begin{cases} l_1 + a_1 - 2 \geq 7 \\ l_2 + b - 3 \leq 6 \\ l_3 + k - 2 \leq 6 \end{cases}$$

It is easy to verify that  $k \leq 6$  and  $b \leq 6$ . If  $b \leq k \leq a \leq 6$ , with similar analysis in Case 6 we can obtain that this lemma holds. Then we consider the case of  $a > 6 \geq k \geq b$ . Without considering graphs with forms  $\Gamma_2(i), \Gamma_2(iii)$  and  $\Gamma_2(iv)$ , we can distinguish this case into the following three subcases.

**Subcase 7.1.**  $k = b = 6, l_1 \geq 3$ .

It is easy to verify that  $l_3 = 2$  and  $2 \leq l_2 \leq 3$ . For any values of  $l_1$  and  $l_2$ , let  $G_{18} \in \Theta_{II}(n; a, 6, 6; l_1, l_2, 2)$  and  $G_{018} \in \Theta_{II}(n; 6, 6, 6; l'_1, l_2, 2)$ , where  $l'_1 = a + l_1 - 6$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{18}) &= b_{2i}(P_{a+l_1+l_2+3}^{a,6} \cup C_6) + b_{2i-2}(P_{a+l_1-2}^a \cup P_{l_2+4}^6 \cup P_5), \\ b_{2i}(G_{018}) &= b_{2i}(P_{a+l_1+l_2+3}^{6,6} \cup C_6) + b_{2i-2}(P_{a+l_1-2}^6 \cup P_{l_2+4}^6 \cup P_5). \end{aligned}$$

By Proposition 2.3, it follows that  $G_{18} \preceq G_{018}$ .

**Subcase 7.2.**  $k = 6, b = 4, l_1 \geq 3$ .

It is easy to verify that  $l_3 = 2$  and  $l_2 \leq 5$ . We have  $4 \leq l_2 \leq 5$  since we do not consider graphs with forms  $\Gamma_2(iii)$  and  $\Gamma_2(iv)$ . For any values of  $l_1$  and  $l_3$ , let  $G_{19} \in \Theta_{II}(n; a, 4, 6; l_1, l_2, 2)$  and  $G_{019} \in \Theta_{II}(n; 6, 6, 6; l'_1, l'_2, 2)$ , where  $l'_1 = a + l_1 - 6$  and  $l'_2 = l_2 - 2$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{19}) &= b_{2i}(P_{a+l_1+l_2+1}^{a,4} \cup C_6) + b_{2i-2}(P_{a+l_1-2}^a \cup P_{l_2+2}^4 \cup P_5), \\ b_{2i}(G_{019}) &= b_{2i}(P_{a+l_1+l_2+1}^{6,6} \cup C_6) + b_{2i-2}(P_{a+l_1-2}^6 \cup P_{l_2+2}^6 \cup P_5). \end{aligned}$$

By Proposition 2.3, we have  $G_{19} \preceq G_{019}$ .

**Subcase 7.3.**  $k = b = 4, l_1 \geq 3, l_3 = 4$ .

Similar to Subcase 7.2, we have  $4 \leq l_2 \leq 5$ . Let  $G_{20} \in \Theta_{II}(n; a, 4, 4; l_1, l_2, 4)$  and  $G_{020} \in \Theta_{II}(n; 6, 6, 6; l'_1, l'_2, 2)$ , where  $l'_1 = a + l_1 - 6$  and  $l'_2 = l_2 - 2$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{20}) &= b_{2i}(P_{a+l_1+l_2+1}^{a,4} \cup P_6^4) + b_{2i-2}(P_{a+l_1-2}^a \cup P_{l_2+2}^4 \cup P_5), \\ b_{2i}(G_{020}) &= b_{2i}(P_{a+l_1+l_2+1}^{6,6} \cup C_6) + b_{2i-2}(P_{a+l_1-2}^6 \cup P_{l_2+2}^6 \cup P_5). \end{aligned}$$

Since  $P_6^4 \prec C_6$  and  $P_5^4 \prec P_5$ , by Proposition 2.3, we have  $G_{20} \preceq G_{020}$ .

$$\text{Case 8. } \begin{cases} l_1 + a - 2 \leq 6 \\ l_2 + b - 3 \leq 6 \\ l_3 + k - 2 \leq 6 \end{cases}$$

It is easy to verify that  $a \leq 6$  and then we have  $b \leq k \leq a \leq 6$ . If  $a = b = k = 6$ , it follows that this lemma holds. Then we focus on other subcases. Without considering the graphs with forms  $\Gamma_2(iii)$  and  $\Gamma_2(iv)$ , we can distinguish this case into the following three subcases.

**Subcase 8.1.**  $a = k = 6, b = 4$ .

It is easy to verify that  $l_1 = l_3 = 2$ . Since  $n \geq 20$ , we have  $l_2 = 5$ . Let  $G_{21} \in \Theta_{II}(20; 6, 4, 6; 2, 5, 2)$  and  $G_{021} \in \Theta_{II}(20; 6, 6, 6; 2, 3, 2)$ . By Lemma 2.2, we have

$$b_{2i}(G_{21}) = b_{2i}(P_{14}^{6,4} \cup C_6) + b_{2i-2}(C_6 \cup P_7^4 \cup P_5),$$

$$b_{2i}(G_{021}) = b_{2i}(P_{14}^{6,6} \cup C_6) + b_{2i-2}(C_6 \cup P_7^6 \cup P_5).$$

By Proposition 2.3, it follows that  $G_{21} \preceq G_{021}$ .

**Subcase 8.2.**  $a = 6, k = b = 4, l_3 = 4$ .

It is easy to verify that  $l_1 = 2, l_2 \leq 5$ . Since  $n \geq 20$ , we have  $l_2 = 5$ . Let  $G_{22} \in \Theta_{II}(20; 6, 4, 4; 2, 5, 4)$  and  $G_{022} \in \Theta_{II}(20; 6, 6, 6; 2, 3, 2)$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{22}) &= b_{2i}(C_6 \cup P_{14}^{4,4}) + b_{2i-2}(P_5 \cup P_6^4 \cup P_7^4), \\ b_{2i}(G_{022}) &= b_{2i}(C_6 \cup P_{14}^{6,6}) + b_{2i-2}(P_5 \cup C_6 \cup P_7^6). \end{aligned}$$

By Proposition 2.3, we have  $G_{22} \preceq G_{022}$ .

**Subcase 8.3.**  $a = k = b = 4, l_1 = l_3 = 4$ .

It is easy to verify that  $l_2 \leq 5$ . Since  $n \geq 20$ , we have  $l_2 = 5$ . Let  $G_{23} \in \Theta_{II}(20; 4, 4, 4; 4, 5, 4)$  and  $G_{023} \in \Theta_{II}(20; 6, 6, 6; 2, 3, 2)$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{23}) &= b_{2i}(P_{13}^{4,4} \cup P_7^4) + b_{2i-2}(P_6^4 \cup P_6^4 \cup P_6^4), \\ b_{2i}(G_{023}) &= b_{2i}(P_{13}^{6,6} \cup P_7^6) + b_{2i-2}(C_6 \cup C_6 \cup C_6). \end{aligned}$$

Since  $P_6^4 \prec C_6$ , and by Proposition 2.3, we can obtain that  $G_{23} \preceq G_{023}$ .

The proof is now complete. ■

**Lemma 3.5** *For any graph  $G \in \Theta_{II}(n; 6, 6, 6; l_1, l_2, l_3)$ , there exists a graph  $H \in \Theta_{II}(n; 6, 6, 6; l'_1, l'_2, 2)$  such that  $G \prec H$ .*

*Proof.* For fixed parameters  $n, l_1, l_2$  and  $l_3$ , let  $G_1 \in \Theta_{II}(n; 6, 6, 6; l_1, l_2, l_3)$  and  $G_0 \in \Theta_{II}(n; 6, 6, 6; l_1, l'_2, 2)$  (as shown in Figure 3.9). It is easy to verify that  $l'_2 = l_2 + l_3 - 2$  and it suffices to show that  $G_1 \prec G_0$ .

By Lemma 2.2 we have

$$\begin{aligned} b_{2i}(G_1) &= b_{2i}(G_1 - u_1v_1) + b_{2i-2}(G_1 - u_1 - v_1) \\ &= b_{2i}(G_1 - u_1v_1) + b_{2i-2}(P_{l_1+3}^6 \cup P_{l_2+4}^6 \cup P_{l_3+4}^6) \\ &= b_{2i}(G_1 - u_1v_1) + b_{2i-2}(P_{l_1+3}^6 \cup P_{l_2+4}^6 \cup C_6 \cup P_{l_3-2}^6) \end{aligned}$$

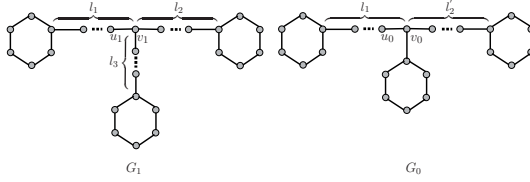


Figure 3.9: Graphs for Lemma 3.5.

$$\begin{aligned}
 & +b_{2i-4}(P_{l_1+3}^6 \cup P_{l_2+4}^6 \cup P_{l_3-3} \cup P_5), \\
 b_{2i}(G_0) & = b_{2i}(G_0 - u_0v_0) + b_{2i-2}(G_0 - u_0 - v_0) \\
 & = b_{2i}(G_0 - u_0v_0) + b_{2i-2}(P_{l_1+3}^6 \cup P_{l_2+l_3+2}^6 \cup C_6) \\
 & = b_{2i}(G_0 - u_0v_0) + b_{2i-2}(P_{l_1+3}^6 \cup P_{l_2+4}^6 \cup C_6 \cup P_{l_3-2}) \\
 & \quad + b_{2i-4}(P_{l_1+3}^6 \cup P_{l_2+3}^6 \cup P_{l_3-3} \cup C_6).
 \end{aligned}$$

Since  $b_{2i}(G_1 - u_1v_1) = b_{2i}(G_0 - u_0v_0)$ , then we only need to compare  $b_{2j}(P_{l_2+4}^6 \cup P_5)$  and  $b_{2j}(P_{l_2+3}^6 \cup C_6)$ . Also by Lemma 2.2 we have

$$\begin{aligned}
 b_{2j}(P_{l_2+4}^6 \cup P_5) & = b_{2j}(P_{l_2+3}^6 \cup P_5 \cup P_1) + b_{2j-2}(P_{l_2+2}^6 \cup P_5) \\
 & = b_{2j}(P_{l_2+3}^6 \cup P_5 \cup P_1) + b_{2j-2}(P_{l_2+2}^6 \cup P_4 \cup P_1) \\
 & \quad + b_{2j-4}(P_{l_2+2}^6 \cup P_3) \\
 & = b_{2j}(P_{l_2+3}^6 \cup P_5 \cup P_1) + b_{2j-2}(P_{l_2+2}^6 \cup P_4 \cup P_1) \\
 & \quad + b_{2j-4}(P_{l_2+1}^6 \cup P_3 \cup P_1) + b_{2j-6}(P_{l_2}^6 \cup P_3) \\
 & = b_{2j}(P_{l_2+3}^6 \cup P_5 \cup P_1) + b_{2j-2}(P_{l_2+2}^6 \cup P_4 \cup P_1) \\
 & \quad + b_{2j-4}(P_{l_2+1}^6 \cup P_3 \cup P_1) + b_{2j-6}(C_6 \cup P_{l_2-6} \cup P_3) \\
 & \quad + b_{2j-8}(P_5 \cup P_{l_2-7} \cup P_3),
 \end{aligned}$$

and

$$\begin{aligned}
 b_{2j}(P_{l_2+3}^6 \cup C_6) & = b_{2j}(P_{l_2+3}^6 \cup P_6) + b_{2j-2}(P_{l_2+3}^6 \cup P_4) + 2b_{2j-6}(P_{l_2+3}^6) \\
 & = b_{2j}(P_{l_2+3}^6 \cup P_6) + b_{2j-2}(P_{l_2+2}^6 \cup P_4 \cup P_1) \\
 & \quad + b_{2j-4}(P_{l_2+1}^6 \cup P_4) + 2b_{2j-6}(P_{l_2+3}^6) \\
 & = b_{2j}(P_{l_2+3}^6 \cup P_6) + b_{2j-2}(P_{l_2+2}^6 \cup P_4 \cup P_1)
 \end{aligned}$$

$$\begin{aligned}
 & +b_{2j-4}(P_{l_2+1}^6 \cup P_3 \cup P_1) + b_{2j-6}(P_{l_2+1}^6 \cup P_2) + 2b_{2j-6}(P_{l_2+3}^6) \\
 = & b_{2j}(P_{l_2+3}^6 \cup P_6) + b_{2j-2}(P_{l_2+2}^6 \cup P_4 \cup P_1) \\
 & +b_{2j-4}(P_{l_2+1}^6 \cup P_3 \cup P_1) + b_{2j-6}(C_6 \cup P_{l_2-5} \cup P_2) \\
 & +b_{2j-8}(P_5 \cup P_{l_2-6} \cup P_2) + 2b_{2j-6}(P_{l_2+3}^6).
 \end{aligned}$$

By Lemma 2.4 and Proposition 2.3 we have  $P_{l_2+4}^6 \cup P_5 \prec P_{l_2+3}^6 \cup C_6$ . Also consider Proposition 2.3, we can obtain that  $G_1 \prec G_0$ . ■

**Lemma 3.6** *For any graph  $G \in \Theta_{II}(n; 6, 6, 6; l_1, l_2, 2)$ , there exists a graph  $H \in \Theta_{II}(n; 6, 6, 6; l, 2, 2)$  such that  $G \prec H$ .*

*Proof.* For fixed parameters  $n$ ,  $l_1$  and  $l_2$ , let  $G_0 \in \Theta_{II}(n; 6, 6, 6; l_1, l_2, 2)$  and  $G_2 \in \Theta_{II}(n; 6, 6, 6; l, 2, 2)$  (as shown in Figure 3.10). It is easy to verify that  $l = l_1 + l_2 - 2$  and it suffices to show that  $G_0 \prec G_2$ .

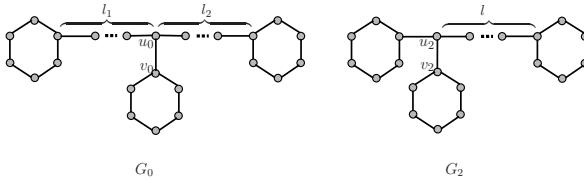


Figure 3.10: Graphs for Lemma 3.6

By Lemma 2.2 we have

$$\begin{aligned}
 b_{2i}(G_0) & = b_{2i}(G_0 - u_0v_0) + b_{2i-2}(G_0 - u_0 - v_0) \\
 & = b_{2i}(G_0 - u_0v_0) + b_{2i-2}(P_{l_1+4}^6 \cup P_{l_2+4}^6 \cup P_5) \\
 & = b_{2i}(G_0 - u_0v_0) + b_{2i-2}(P_{l_2+4}^6 \cup C_6 \cup P_{l_1-2} \cup P_5) \\
 & \quad + b_{2i-4}(P_{l_2+4}^6 \cup P_5 \cup P_{l_1-3} \cup P_5), \\
 b_{2i}(G_2) & = b_{2i}(G_2 - u_2v_2) + b_{2i-2}(G_2 - u_2 - v_2) \\
 & = b_{2i}(G_2 - u_2v_2) + b_{2i-2}(P_{l_1+l_2+2}^6 \cup C_6 \cup P_5) \\
 & = b_{2i}(G_2 - u_2v_2) + b_{2i-2}(P_{l_2+4}^6 \cup C_6 \cup P_{l_1-2} \cup P_5)
 \end{aligned}$$

$$+b_{2i-4}(P_{l_2+3}^6 \cup C_6 \cup P_{l_1-3} \cup P_5).$$

Since  $b_{2i}(G_0 - u_0v_0) = b_{2i}(G_2 - u_2v_2)$ , then we only need to compare  $b_{2j}(P_{l_2+4}^6 \cup P_5)$  with  $b_{2j}(P_{l_2+3}^6 \cup C_6)$ . With similar analysis in Lemma 3.5, we can obtain that  $G_0 \prec G_2$ .

■

From Theorem 3.4, Lemmas 3.5 and 3.6, we can easily obtain the following result.

**Theorem 3.7** *For any graph  $G \in \Theta_{II}(n; a, b, k; l_1, l_2, l_3)$ , if  $G$  is not an element of the special graph class  $\Gamma_2$ , then there exists a graph  $H \in \Theta_{II}(n; 6, 6, 6; n - 17, 2, 2)$  such that  $G \preceq H$ , and the equality holds if and only if  $G \cong H$ .*

**Theorem 3.8** *For any graph  $G \in \Theta_I(n; a, b, k; l_1, l_2; 2) \setminus \Gamma_1$ , there exists a graph  $H \in \Theta_I(n; 6, 6, 6; l'_1, l'_2; 2)$  such that  $G \preceq H$ .*

*Proof.* Without loss of generality, we may assume that  $l_1 \geq l_2$ . We will discuss the following four cases.

$$\text{Case 1. } \begin{cases} l_1 + a - 1 \geq 9 \\ l_2 + k - 1 \geq 8 \end{cases}$$

Considering the values of  $l_1$  and  $l_2$ , we distinguish this case into the following four subcases.

**Subcase 1.1.**  $l_1 \geq 4$ .

For any values of  $l_1$  and  $l_2$ , let  $G_1 \in \Theta_I(n; a, b, k; l_1, l_2; 2)$  and  $G_{01} \in \Theta_I(n; 6, 6, 6; l'_1, l'_2; 2)$ , where  $l'_1 = a + l_1 - 6$ . By lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_1) &= b_{2i}(P_{a+l_1-2}^a \cup P_{b+k+l_2-2}^{b,k}) + b_{2i-2}(P_{a+l_1-3}^a \cup P_{b+k+l_2-3}^k), \\ b_{2i}(G_{01}) &= b_{2i}(P_{a+l_1-2}^6 \cup P_{b+k+l_2-2}^{6,6}) + b_{2i-2}(P_{a+l_1-3}^6 \cup P_{b+k+l_2-3}^6). \end{aligned}$$

By Proposition 2.3, we can obtain that  $G_1 \preceq G_{01}$ .

**Subcase 1.2.**  $l_1 = l_2 = 3$  and  $b \geq 6$ .

It is easy to verify that  $a \geq 8$  and  $k \geq 6$ . Let  $G_2 \in \Theta_I(n; a, b, k; 3, 3; 2)$  and  $G_{02} \in \Theta_I(n; 6, 6, 6; l'_1, l'_2; 2)$ , where  $l'_1 = a - 3$  and  $l'_2 = b + k - 9$ . By lemma 2.2, we have

$$b_{2i}(G_2) = b_{2i}(P_n^{a,k}) + b_{2i-2}(P_{a+1}^a \cup P_{k+1}^k \cup P_{b-2}) + (-1)^{1+\frac{i}{2}} 2b_{2i-b}(P_{a+1}^a \cup P_{k+1}^k),$$



$$b_{2i}(G_{02}) = b_{2i}(P_n^{6,6}) + b_{2i-2}(P_{a+1}^6 \cup P_{b+k-5}^6 \cup P_4) + 2b_{2i-6}(P_{a+1}^6 \cup P_{b+k-5}^6).$$

Then we compare  $b_{2j}(P_{k+1}^k \cup P_{b-2})$  with  $b_{2j}(P_{b+k-5}^6 \cup P_4)$ . By Lemma 2.2 we have

$$\begin{aligned} b_{2j}(P_{k+1}^k \cup P_{b-2}) &= b_{2j}(P_{k+1} \cup P_{b-2}) + b_{2j-2}(P_{k-2} \cup P_{b-2} \cup P_1), \\ b_{2j}(P_{b+k-5}^6 \cup P_4) &= b_{2j}(P_{b+k-5} \cup P_4) + b_{2j-2}(P_{b+k-11} \cup P_4 \cup P_4). \end{aligned}$$

Since  $b \geq 6$  and  $k \geq 6$ , by Lemma 2.4, we have  $P_{k+1} \cup P_{b-2} \prec P_{b+k-5} \cup P_4$  and  $P_{k-2} \cup P_{b-2} \cup P_1 \prec P_{k-2} \cup P_{b-5} \cup P_4 \preceq P_{b+k-11} \cup P_4 \cup P_4$ . Then we can obtain that  $P_{k+1}^k \cup P_{b-2} \preceq P_{b+k-5}^6 \cup P_4$ . Also, since  $b \geq 6$ , then  $k+1 \leq b+k-5$ , by Proposition 2.3 we have  $P_{k+1}^k \preceq P_{k+1}^6 \preceq P_{b+k-5}^6$ . Also by Proposition 2.3, we can obtain that  $G_2 \preceq G_{02}$ .

**Subcase 1.3.**  $l_1 = l_2 = 3$ ,  $b = 4$  and  $k = 6$ .

It is easy to verify that  $a \geq 8$ . Let  $G_3 \in \Theta_I(n; a, 4, 6; 3, 3; 2)$  and  $G_{03} \in \Theta_I(n; 6, 6, 6; l'_1, 3; 2)$ , where  $l'_1 = a - 5$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_3) &= b_{2i}(P_{a+5}^{a,4} \cup P_7^6) + b_{2i-2}(P_{a+4}^a \cup C_6), \\ b_{2i}(G_{03}) &= b_{2i}(P_{a+5}^{6,6} \cup P_7^6) + b_{2i-2}(P_{a+4}^6 \cup C_6). \end{aligned}$$

From Proposition 2.3, it follows that  $G_3 \preceq G_{03}$ .

**Subcase 1.4.**  $l_1 = l_2 = 3$ ,  $b = 4$ ,  $k \geq 8$  or  $l_1 = 3$ ,  $l_2 = 2$  or  $l_1 = l_2 = 2$ .

The graphs in this case belong to  $\Gamma_1(i)$  or  $\Gamma_1(ii)$ , so we do not consider them.

$$\text{Case 2. } \begin{cases} l_1 + a - 1 \leq 8 \\ l_2 + k - 1 \geq 8 \end{cases}$$

It is easy to verify that  $a \leq 6$ . Without considering graphs of form  $\Gamma_1(iii)$ , we distinguish this case into the following two subcases.

**Subcase 2.1.**  $a = 6$ .

It is easy to verify that  $l_1 = 2$  or  $3$ . If  $l_1 = 3$ ,  $l_2 = 3$ , then let  $G_4 \in \Theta_I(n; 6, b, k; 3, 3; 2)$  and  $G_{04} = \Theta_I(n; 6, 6, 6; 3, l'_2; 2)$ , where  $l'_2 = b + k - 9$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_4) &= b_{2i}(P_{b+k+1}^{b,k} \cup P_7^6) + b_{2i-2}(P_{b+k}^k \cup C_6), \\ b_{2i}(G_{04}) &= b_{2i}(P_{b+k+1}^{6,6} \cup P_7^6) + b_{2i-2}(P_{b+k}^6 \cup C_6). \end{aligned}$$

By Proposition 2.3, we have  $G_4 \preceq G_{04}$ .

If  $l_1 = 3$ ,  $l_2 = 2$ , then let  $G_5 \in \Theta_I(n; 6, b, k; 3, 2; 2)$  and  $G_{05} = \Theta_I(n; 6, 6, 6; 3, l_2''; 2)$ , where  $l_2'' = b + k - 10$ . With similar analysis, it follows that  $G_5 \preceq G_{05}$ . If  $l_1 = l_2 = 2$ , then let  $G_6 \in \Theta_I(n; 6, b, k; 2, 2; 2)$  and  $G_{06} \in \Theta_I(n; 6, 6, 6; 2, l_2''; 2)$ , where  $l_2'' = b + k - 10$ . With similar analysis, we can obtain that  $G_6 \preceq G_{06}$ .

**Subcase 2.2.**  $a = 4$ :

It is easy to verify that  $l_1 \leq 5$ . Since we do not consider graphs with form  $\Gamma_1(iii)$ , we have  $4 \leq l_1 \leq 5$ . If  $l_1 = 5$ , let  $G_7 \in \Theta_I(n; 4, b, k; 5, l_2; 2)$  and  $G_{07} \in \Theta_I(n; 6, 6, 6; 3, l_2'; 2)$ , where  $l_2' = b + k + l_2 - 12$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_7) &= b_{2i}(P_{b+k+l_2-2}^{b,k} \cup P_7^4) + b_{2i-2}(P_{b+k+l_2-3}^k \cup P_6^4), \\ b_{2i}(G_{07}) &= b_{2i}(P_{b+k+l_2-2}^{6,6} \cup P_7^6) + b_{2i-2}(P_{b+k+l_2-3}^6 \cup C_6). \end{aligned}$$

From Proposition 2.3, it follows that  $G_7 \preceq G_{07}$ . If  $l_1 = 4$ , let  $G_8 \in \Theta_I(n; 4, b, k; 4, l_2; 2)$  and  $G_{08} \in \Theta_I(n; 6, 6, 6; 2, l_2'; 2)$ , where  $l_2' = b + k + l_2 - 12$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_8) &= b_{2i}(P_{b+k+l_2-2}^{b,k} \cup P_6^4) + b_{2i-2}(P_{b+k+l_2-3}^k \cup P_5^4), \\ b_{2i}(G_{08}) &= b_{2i}(P_{b+k+l_2-2}^{6,6} \cup C_6) + b_{2i-2}(P_{b+k+l_2-3}^6 \cup P_5). \end{aligned}$$

Since  $P_5^4 \prec P_5$ , then from Proposition 2.3, it follows that  $G_8 \preceq G_{08}$ .

$$\text{Case 3. } \begin{cases} l_1 + a - 1 \geq 9 \\ l_2 + k - 1 \leq 7 \end{cases}$$

Without considering graphs with form  $\Gamma_1(iv)$ , we distinguish this case into the following two subcases.

**Subcase 3.1.**  $k = 6$ .

It is easy to verify that  $l_2 = 2$ . For any value of  $l_1$ , let  $G_9 \in \Theta_I(n; a, b, 6; l_1, 2; 2)$  and  $G_{09} \in \Theta_I(n; 6, 6, 6; l_1', 2; 2)$ , where  $l_1' = a + b + l_1 - 12$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_9) &= b_{2i}(P_{a+b+l_1-2}^{a,b} \cup C_6) + b_{2i-2}(P_{a+b+l_1-3}^a \cup P_5), \\ b_{2i}(G_{09}) &= b_{2i}(P_{a+b+l_1-2}^{6,6} \cup C_6) + b_{2i-2}(P_{a+b+l_1-3}^6 \cup P_5). \end{aligned}$$

By Proposition 2.3, we can obtain that  $G_9 \preceq G_{09}$ .

**Subcase 3.2.**  $k = 4$ .

It is easy to verify that  $l_2 \leq 4$ . Since we do not consider graphs with form  $\Gamma_1(iv)$ , we have  $l_2 = 4$ . For any value of  $l_1$ , let  $G_{10} \in \Theta_I(n; a, b, 4; l_1, 4; 2)$  and  $G_{010} \in \Theta_I(n; 6, 6, 6; l'_1, 2; 2)$ , where  $l'_1 = a + b + l_1 - 12$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{10}) &= b_{2i}(P_{a+b+l_1-2}^{a,b} \cup P_6^4) + b_{2i-2}(P_{a+b+l_1-3}^a \cup P_5^4), \\ b_{2i}(G_{010}) &= b_{2i}(P_{a+b+l_1-2}^{6,6} \cup C_6) + b_{2i-2}(P_{a+b+l_1-3}^6 \cup P_5^6). \end{aligned}$$

Since  $P_5^4 \prec P_5$ , by Proposition 2.3, we can obtain that  $G_{10} \preceq G_{010}$ .

**Case 4.**  $\begin{cases} l_1 + a - 1 \leq 8 \\ l_2 + k - 1 \leq 7 \end{cases}$

It is easy to verify that  $a \leq 6$  and  $k \leq 6$ . Without considering graphs with form  $\Gamma_1(v)$ , we distinguish this case into the following two subcases.

**Subcase 4.1.**  $a = 6$ :

It is easy to verify that  $l_1 \leq 3$ . If  $l_1 = 3$ , then let  $G_{11} \in \Theta_I(n; 6, b, k; 3, l_2; 2)$  and  $G_{011} \in \Theta_I(n; 6, 6, 6; 3, l'_2; 2)$ , where  $l'_2 = b + k + l_2 - 12$ . By Lemma 2.2, we have

$$\begin{aligned} b_{2i}(G_{11}) &= b_{2i}(P_{b+k+l_2-2}^{b,k} \cup P_7^6) + b_{2i-2}(P_{b+k+l_2-3}^k \cup C_6), \\ b_{2i}(G_{011}) &= b_{2i}(P_{b+k+l_2-2}^{6,6} \cup P_7^6) + b_{2i-2}(P_{b+k+l_2-3}^6 \cup C_6). \end{aligned}$$

By Proposition 2.3, we can obtain that  $G_{11} \preceq G_{011}$ .

If  $l_1 = 2$ , since  $l_1 \geq l_2$ , we have  $l_2 = 2$ . Let  $G_{12} \in \Theta_I(n; 6, b, k; 2, 2; 2)$  and  $G_{012} \in \Theta_I(n; 6, 6, 6; 2, l'_2; 2)$ , where  $l'_2 = b + k - 10$ . With similar analysis, it follows that  $G_{12} \preceq G_{012}$ .

**Subcase 4.2.**  $a = 4$ .

It is easy to verify that  $l_1 \leq 5$ . Since we do not consider graphs with form  $\Gamma_1(iv)$ , then we have  $4 \leq l_1 \leq 5$ . If  $l_1 = 5$ , then let  $G_{13} \in \Theta_I(n; 4, b, k; 5, l_2; 2)$  and  $G_{013} \in \Theta_I(n; 6, 6, 6; 3, l'_2; 2)$ , where  $l'_2 = b + k + l_2 - 12$ . By Lemma 2.2, we have  $b_{2i}(G_{13}) = b_{2i}(P_{b+k+l_2-2}^{b,k} \cup P_7^4) + b_{2i-2}(P_{b+k+l_2-3}^k \cup P_6^4)$  and  $b_{2i}(G_{013}) = b_{2i}(P_{b+k+l_2-2}^{6,6} \cup P_7^6) + b_{2i-2}(P_{b+k+l_2-3}^6 \cup C_6)$ . By Proposition 2.3, we can obtain that  $G_{13} \preceq G_{013}$ .

If  $l_1 = 4$ , then let  $G_{14} \in \Theta_I(n; 4, b, k; 4, l_2; 2)$  and  $G_{014} = \Theta_I(n; 6, 6, 6; 2, l'_2; 2)$ , where  $l'_2 = b + k + l_2 - 12$ . With similar analysis we can obtain that  $G_{14} \preceq G_{014}$ .

The proof is thus complete. ■

**Lemma 3.9** *For any graph  $G \in \Theta_I(n; 6, 6, 6; l_1, l_2; 2)$ , there exists a graph  $H \in \Theta_I(n; 6, 6, 6; l'_1, 2; 2)$  such that  $G \prec H$ .*

*Proof.* For fixed parameters  $n, a, b, k, l_1$  and  $l_2$ , let  $G_1 \in \Theta_I(n; a, b, k; l_1, l_2; 2)$  and  $G_0 = \Theta_I(n; a, b, k; l'_1, 2; 2)$  (as shown in Figure 3.11). It is easy to verify that  $l'_1 = l_1 + l_2 - 2$  and it suffices to show that  $G_1 \prec G_0$ .

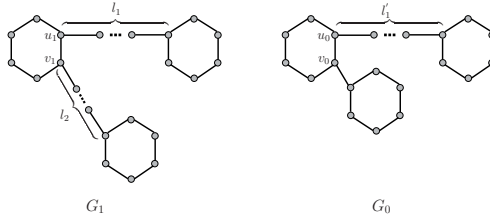


Figure 3.11: Graphs for Lemma 3.9.

By Lemma 2.2 we have

$$\begin{aligned}
 b_{2i}(G_1) &= b_{2i}(G_1 - u_1 v_1) + b_{2i-2}(G_1 - u_1 - v_1) + 2b_{2i-6}(G_1 - C_6) \\
 &= b_{2i}(G_1 - u_1 v_1) + b_{2i-2}(P_{l_1+4}^6 \cup P_{l_2+4}^6 \cup P_4) + 2b_{2i-6}(P_{l_1+4}^6 \cup P_{l_2+4}^6), \\
 b_{2i}(G_0) &= b_{2i}(G_0 - u_0 v_0) + b_{2i-2}(G_2 - u_0 - v_0) + 2b_{2i-6}(G_0 - C_6) \\
 &= b_{2i}(G_0 - u_0 v_0) + b_{2i-2}(P_{l'_1+4}^6 \cup C_6 \cup P_4) + 2b_{2i-6}(P_{l'_1+4}^6 \cup C_6).
 \end{aligned}$$

Since  $b_{2i}(G_1 - u_1 v_1) = b_{2i}(G_0 - u_0 v_0)$ , and considering Proposition 2.3, we try to compare  $b_{2j}(P_{l_1+4}^6 \cup P_{l_2+4}^6)$  with  $b_{2j}(P_{l'_1+4}^6 \cup C_6)$ . Also by Lemma 2.2 we have

$$\begin{aligned}
 b_{2j}(P_{l_1+4}^6 \cup P_{l_2+4}^6) &= b_{2j}(P_{l_1+4}^6 \cup C_6 \cup P_{l_2-2}) + b_{2j-2}(P_{l_1+4}^6 \cup P_{l_2-3} \cup P_5), \\
 b_{2j}(P_{l'_1+4}^6 \cup C_6) &= b_{2j}(P_{l_1+4}^6 \cup C_6 \cup P_{l_2-2}) + b_{2j-2}(P_{l_1+3}^6 \cup P_{l_2-3} \cup C_6).
 \end{aligned}$$

With similar analysis in Lemma 3.5, we have  $P_{l_1+4}^6 \cup P_5 \prec P_{l_1+3}^6 \cup C_6$ . Applying Proposition 2.3, we can obtain  $G_1 \prec G_0$ . ■

**Lemma 3.10** For any graph  $G \in \Theta_I(n; 6, 6, 6; l_1, 2; 2)$ , there exists a graph  $H \in \Theta_{II}(n; 6, 6, 6; l, 2, 2)$  such that  $\mathcal{E}(G) < \mathcal{E}(H)$ .

*Proof.* For fixed parameters  $l_1$  and  $l$ , let  $G_0 \in \Theta_I(n; 6, 6, 6; l_1, 2; 2)$  and  $G_2 \in \Theta_{II}(n; 6, 6, 6; l, 2, 2)$  (as shown in Figure 3.12), where  $l = l_1 - 1$ , i.e.,  $l_1 = l + 1$ . It suffices to show that  $G_0 \prec G_2$ .

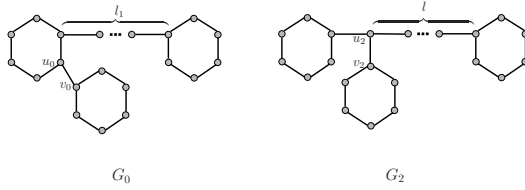


Figure 3.12: Graphs for Lemma 3.10.

By Lemma 2.2 we have

$$\begin{aligned}
 b_{2i}(G_0) &= b_{2i}(G_0 - u_0v_0) + b_{2i-2}(G_0 - u_0 - v_0) \\
 &= b_{2i}(G_0 - u_0v_0) + b_{2i-2}(P_{l+10}^6 \cup P_5) \\
 &= b_{2i}(G_0 - u_0v_0) + b_{2i-2}(P_{l+4}^6 \cup P_6 \cup P_5) + b_{2i-4}(P_{l+3}^6 \cup P_5 \cup P_5), \\
 b_{2i}(G_2) &= b_{2i}(G_2 - u_2v_2) + b_{2i-2}(G_2 - u_2 - v_2) \\
 &= b_{2i}(G_2 - u_2v_2) + b_{2i-2}(P_{l+4}^6 \cup C_6 \cup P_5) \\
 &= b_{2i}(G_2 - u_2v_2) + b_{2i-2}(P_{l+4}^6 \cup P_6 \cup P_5) + b_{2i-4}(P_{l+4}^6 \cup P_4 \cup P_5).
 \end{aligned}$$

Since  $b_{2i}(G_0 - u_0v_0) = b_{2i}(G_2 - u_2v_2)$ , then we only need to verify  $P_{l+3}^6 \cup P_5 \cup P_5 \prec P_{l+4}^6 \cup P_4 \cup P_5$ . By Lemma 2.2, we have

$$\begin{aligned}
 b_{2i}(P_{l+3}^6 \cup P_5) &= b_{2i}(P_{l+3} \cup P_5) + b_{2i-2}(P_{l-3} \cup P_5 \cup P_4) + 2b_{2i-6}(P_{l-3} \cup P_5), \\
 b_{2i}(P_{l+4}^6 \cup P_4) &= b_{2i}(P_{l+4} \cup P_4) + b_{2i-2}(P_{l-2} \cup P_4 \cup P_4) + 2b_{2i-6}(P_{l-2} \cup P_4).
 \end{aligned}$$

From Lemma 2.4, we can obtain that  $P_{l+3} \cup P_5 \prec P_{l+4} \cup P_4$  and if  $l \neq 5$ ,  $P_{l-3} \cup P_5 \prec P_{l-2} \cup P_4$ , then  $P_{l-3} \cup P_5 \cup P_4 \prec P_{l-2} \cup P_4 \cup P_4$ . So from Proposition 2.3, it follows that  $P_{l+3}^6 \cup P_5 \prec P_{l+4}^6 \cup P_4$  and then  $G_0 \prec G_2$ . If  $l = 5$ , then  $G_0 \in \Theta_I(22; 6, 6, 6; 6, 2; 2)$  and  $G_2 \in \Theta_{II}(22; 6, 6, 6; 5, 2, 2)$ . By calculating, we know that  $\mathcal{E}(G_0) < \mathcal{E}(G_2)$ .

Therefore, the proof is complete. ■

From Theorem 3.8 and Lemmas 3.3, 3.9 and 3.10, we can easily obtain the following theorem.

**Theorem 3.11** *For any graph  $G \in \Theta_I(n; a, b, k; l_1, l_2; l_c)$  and  $G \notin \Gamma_1$ , there exists a graph  $H \in \Theta_{II}(n; 6, 6, 6; n - 17, 2, 2)$  such that  $G \preceq H$ , and the equality holds if and only if  $G \cong H$ .*

From Theorems 3.7 and 3.11, we can obtain our main result Theorem 2.5.

## References

- [1] E. O. D. Andriantiana, Unicyclic bipartite graphs with maximum energy, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 913–926.
- [2] E. O. D. Andriantiana, S. Wagner, Unicyclic graphs with large energy, *Lin. Algebra Appl.* **435** (2011) 1399–1414.
- [3] M. Aouchiche, G. Caporossi, P. Hansen, Open problems on graph eigenvalues studied with AutoGraphiX, *Europ. J. Comput. Optim.* **1** (2013) 181–199.
- [4] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, New York, 2008.
- [5] G. Caporossi, D. Cvetković, I. Gutman, P. Hansen, Variable neighborhood search for extremal graphs. 2. Finding graphs with extremal energy, *J. Chem. Inf. Comput. Sci.* **39** (1999) 984–996.
- [6] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, Academic Press, New York, 1980.
- [7] B. Furtula, S. Radenković, I. Gutman, Bicyclic molecular graphs with the greatest energy, *J. Serb. Chem. Soc.* **73** (2008) 431–433.
- [8] I. Gutman, Acyclic systems with extremal Hückel  $\pi$ -electron energy, *Theor. Chim. Acta* **45** (1977) 79–87.

- [9] 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, Berlin, 2001, pp. 196–211.
- [10] I. Gutman, X. Li, J. Zhang, Graph energy, in: M. Dehmer, F. Emmert-Streib (Eds.), *Analysis of Complex Networks: From Biology to Linguistics*, Wiley-VCH, Weinheim, 2009, pp. 145–174.
- [11] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.
- [12] I. Gutman, D. Vidović, Quest for molecular graphs with maximal energy: a computer experiment, *J. Chem. Inf. Sci.* **41** (2001) 1002–1005.
- [13] Y. Hou, Unicyclic graphs with minimal energy, *J. Math. Chem.* **29** (2001) 163–168.
- [14] Y. Hou, Bicyclic graphs with minimal energy, *Lin. Multilin. Algebra.* **49** (2001) 347–354.
- [15] Y. Hou, I. Gutman, C. Woo, Unicyclic graphs with maximal energy, *Lin. Algebra Appl.* **356** (2002) 27–36.
- [16] B. Huo, J. Ji, X. Li, Note on unicyclic graphs with given number of pendant vertices and minimal energy, *Lin. Algebra Appl.* **433** (2010) 1381–1387.
- [17] B. Huo, J. Ji, X. Li, Solutions to unsolved problems on the minimal energies of two classes of graphs, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 943–958.
- [18] B. Huo, J. Ji, X. Li, Y. Shi, Complete solution to a conjecture on the fourth maximal energy tree, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 903–912.
- [19] B. Huo, S. Ji, X. Li, Y. Shi, Solution to a conjecture on the maximal energy of bipartite bicyclic graphs, *Lin. Algebra Appl.* **435** (2011) 804–810.
- [20] B. Huo, X. Li, Y. Shi, Complete solution to a problem on the maximal energy of unicyclic bipartite graphs, *Lin. Algebra Appl.* **434** (2011) 1370–1377.

- [21] B. Huo, X. Li, Y. Shi, Complete solution to a conjecture on the maximal energy of unicyclic graphs, *Eur. J. Combin.* **32** (2011) 662–673.
- [22] B. Huo, X. Li, Y. Shi, L. Wang, Determining the conjugated trees with the third through the sixth minimal energies, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 521–532.
- [23] F. Li, B. Zhou, Minimal energy of bipartite unicyclic graphs of a given bipartition, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 379–388.
- [24] S. Li, X. Li, On tetracyclic graphs with minimal energy, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 395–414.
- [25] S. Li, N. Li, On minimal energies of acyclic conjugated molecules, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 341–349.
- [26] S. Li, X. Li, On tricyclic graphs of a given diameter with minimal energy, *Lin. Algebra Appl.* **430** (2009) 370–385.
- [27] S. Li, X. Li, Z. Zhou, On tricyclic graphs with minimal energy, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 397–419.
- [28] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2012.
- [29] X. Li, J. Zhang, On bicyclic graphs with maximal energy, *Lin. Algebra Appl.* **427** (2007) 87–98.
- [30] X. Li, J. Zhang, L. Wang, On bipartite graphs with minimal energy, *Discr. Appl. Math.* **157** (2009) 869–873.
- [31] S. Wagner, Energy bounds for graphs with fixed cyclomatic number, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 661–674.
- [32] F. Zhang, H. Li, On acyclic conjugated molecules with minimal energy, *Discr. Appl. Math.* **92** (1999) 71–84.