# Bipartite Unicyclic Graphs with Large Energy 

Hongbo Hua<br>Department of Computing Science, Huaiyin Institute of Technology, Huaian, Jiangsu 223000, People's Republic of China<br>email: hongbo.hua@gmail.com

(Received February 12, 2007)


#### Abstract

Let $G$ be a graph with $n$ vertices and $\lambda_{1}, \lambda_{2}, \cdots, \lambda_{n}$ be $n$ eigenvalues of its adjacency matrix $A(G)$. The energy of $G$, denoted by $E(G)$, is defined to be the summation $\sum_{i=1}^{n}\left|\lambda_{i}\right|$. Denote by $\mathcal{B} \mathcal{U}_{n}$ the set of connected bipartite unicyclic graphs on $n$ vertices. For $n \geq l+1$, let $P_{n}^{l}$ be graph obtained by identifying one pendent vertex of the path $P_{n-l+1}$ with any vertex of the cycle $C_{l}$. Recently, I. Gutman ${ }^{[7]}$ and Y. Hou ${ }^{[10]}$ determined that $P_{n}^{6}$ is the unique graph with the greatest energy among all graphs in $\mathcal{B} \mathcal{U}_{n} \backslash\left\{C_{n}\right\}$. Let $\mathcal{B} \mathcal{U}^{*}{ }_{n}=\mathcal{B} \mathcal{U}_{n} \backslash\left\{C_{n}, P_{n}^{l}, l=4,5, \cdots, n-1\right\}$. It is proved in this paper that for $n \geq 13, M_{n}^{6,3}$ is the graph with maximal energy among all graphs in $\mathcal{B} \mathcal{U}^{*}{ }_{n}$, where $M_{n}^{6,3}$ is the graph obtained by joining (by a new edge ) any vertex of the hexagon with the vertex 3 of the path $P_{n-6}$.


## 1 Introduction

Let $G$ be a connected graph with $n$ vertices and $A(G)$ be its adjacency matrix. The characteristic polynomial of $A(G)$ is defined to be

$$
\phi(G ; x)=|x I-A(G)|=\sum_{i=0}^{n} a_{i} x^{n-i},
$$

which is also said to be the characteristic polynomial of $G$. All $n$ roots $\lambda_{1}, \lambda_{2}, \cdots, \lambda_{n}$ of $\phi(G ; x)$ are called to be eigenvalues of $G$. It's not difficult to see that each $\lambda_{i}(i=1,2, \cdots n)$ is real since $A(G)$ is symmetric.

The energy of $G$, denoted by $E(G)$, is defined to be $\sum_{i=1}^{n}\left|\lambda_{i}\right|$. It's well known that $E(G)$ can
be expressed as the coulson integral formula

$$
\begin{equation*}
E(G)=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} \frac{1}{x^{2}} \ln \left[\left(\sum_{i=0}^{\left\lfloor\frac{n}{2}\right\rfloor}(-1)^{i} a_{2 i} x^{2 i}\right)^{2}+\left(\sum_{i=0}^{\left\lfloor\frac{n}{2}\right\rfloor}(-1)^{i} a_{2 i+1} x^{2 i+1}\right)^{2}\right] d x \tag{1}
\end{equation*}
$$

where $a_{0}, a_{1} \cdots, a_{n}$ are coefficients of characteristic polynomial of $G$.
Since the energy of a graph can be used to estimate approximately the total $\pi$-electron energy of the molecule, it has been intensively studied by many scholars. For more details see [3-10]; for some recent research along these lines see [11-22]. The interested reader may also refer to $[23,24]$ for the mathematical properties of $E(G)$.

As usual, we begin with some notations and terminologies. For a graph $G$, we use $V(G)$ and $E(G)$ to denote its set of vertices and edges, respectively. Let $d_{G}(v)$ denote the degree of vertex $v$, namely the number of edges incident with $v$ in $G$. By $d_{G}(x, y)$ we mean the length of the shortest path connecting vertices $x$ and $y$, i.e., the distance between $x$ and $y$ in $G$. Let $V_{p}(G)$ denote the set of pendent vertices in $G$. By $S_{n}, C_{n}$ and $P_{n}$ we denote respectively the star graph, the cycle graph and the path graph with n vertices. Let $P_{n}^{l}(n \geq l+1)$ be graph obtained by identifying one pendent vertex of the path $P_{n-l+1}$ with any vertex of the cycle $C_{l}$. Denote by $K_{n}^{l}(n \geq l+2)$ the graph obtained from $P_{n-1}^{l}$ by attaching one pendent edge to one neighbor (lying on $C_{l}$ ) of the unique 3-degree vertex of $P_{n-1}^{l}$. By $R_{n}^{l}(n \geq l+4)$ we denote the graph obtained by attaching a path of length 2 to one neighbor (lying on $C_{l}$ ) of the unique 3 -degree vertex of $P_{n-2}^{l}$. Let $Q_{n}^{l}(n \geq l+5)$ be graph obtained by identifying the middle-point of the path $P_{5}$ with the unique pendent vertex of $P_{n-4}^{l}$. Fig.1. illustrate $P_{n}^{l}, K_{n}^{l}, R_{n}^{l}$ and $Q_{n}^{l}$, respectively.


Fig.1.
Denote by $\mathcal{U}_{n}$ and $\mathcal{B} \mathcal{U}_{n}$ the set of connected unicyclic graphs and bipartite unicyclic graphs on $n$ vertices, respectively. Let $G$ be any graph in $\mathcal{U}_{n}$ and $v$ the vertex lying on its unique
cycle. If $d_{G}(v) \geq 3$, then $v$ is said to be a branched vertex. For a given vertex $x \notin V\left(C_{l}\right)$ in $G$, let $d_{G}\left(x, C_{l}\right)=\min \left\{d_{G}(x, y) \mid y \in V\left(C_{l}\right)\right\}$, where $C_{l}$ is the cycle in $G$.

 $V_{p}(G)$ such that $\left.d_{G}\left(x, C_{l}\right)=1\right\}$. Set $\mathcal{B} \mathcal{U}^{*}{ }_{n, 2}=\mathcal{B U}^{*}{ }_{n} \backslash \mathcal{B U}^{*}{ }_{n, 1}$. Let $\mathcal{B} \mathcal{U}^{*}{ }_{n, 2}$ denote the subset of $\mathcal{B U}^{*}{ }_{n, 2}$ such that for any $G \in \mathcal{B U}^{*}{ }_{n, 2}$, there's exactly one branched vertex in the unique cycle of $G$. Denote by $\mathcal{B U}^{* a}{ }_{n, 2}$ the set $\mathcal{B \mathcal { U } ^ { * } { } _ { n , 2 } \backslash \mathcal { B } \mathcal { U } ^ { * b } { } _ { n , 2 } \text { . By } \mathcal { B } \mathcal { U } ^ { * b } { } _ { n , 2 } ( l ) \text { we mean the subset of } \mathcal { B } \mathcal { U } ^ { * b } { } _ { n , 2 } , ~}$ such that for each graph $G$ in $\mathcal{B U}_{n, 2}^{* b}(l), G$ has a unique cycle of length $l$. Similarly, we can define respectively the sets $\mathcal{B} \mathcal{U}^{*}{ }_{n}(l), \mathcal{B} \mathcal{U}_{n, 2}^{* a}(l), \mathcal{U}_{n}(l)$ and $\mathcal{B} \mathcal{U}_{n}(l)$ in this way.

In this paper, we determined the graph with maximal energy among all graphs in $\mathcal{B} \mathcal{U}^{*}{ }_{n}$.

## 2 Lemmas and Results

Sachs theorem [25] states that

$$
\begin{equation*}
a_{i}(G)=\sum_{S \in L_{i}}(-1)^{k(S)} 2^{c(S)}, \tag{2}
\end{equation*}
$$

where $L_{i}$ denote the set of Sachs graphs $G$ with $i$ vertices, $k(S)$ is number of components of $S$ and $c(S)$ is the number of cycles contained in $S$.

Set $b_{i}(G)=\left|a_{i}(G)\right|(i=0,1 \cdots, n)$. From Eq.(2), we find that $b_{2}(G)$ is equal to the number of edges of $G$. Let $m(G, k)$ denote the number of $k$-matchings of a graph $G$. If $G$ contains no cycle, then $b_{2 k}(G)=m(G, k)$ and $b_{2 k+1}(G)=0$ for each $k \geq 0$. It's both consistent and convenient to define $b_{k}(G)=0$ and $m(G ; k)=0$ for the case when $k<0$.

In [8], Y. Hou obtained the following result.

Lemma 1. Let $G \in \mathcal{U}_{n}(l)$. Then $(-1)^{k} a_{2 k} \geq 0$ for all $k \geq 0$; and $(-1)^{k} a_{2 k+1} \geq 0$ (resp. $\leq 0)$ for all $k \geq 0$ if $l=2 r+1$ and $r$ is odd (resp. even ).

From Eq.(1) and lemma 1, we obtain

$$
\begin{equation*}
E(G)=\frac{1}{\pi} \int_{0}^{+\infty} \frac{1}{x^{2}} \ln \left[\left(\sum_{i=0}^{\left\lfloor\frac{n}{2}\right\rfloor} b_{2 i} x^{2 i}\right)^{2}+\left(\sum_{i=0}^{\left\lfloor\frac{n}{2}\right\rfloor} b_{2 i+1} x^{2 i+1}\right)^{2}\right] d x \tag{3}
\end{equation*}
$$

It follows from (3) that $E(G)$ is a strictly increasing function of $b_{i}(G)$ for $i=0,1, \cdots, n$. That is to say, for any two unicyclic graphs $G_{1}$ and $G_{2}$, there exists

$$
\begin{equation*}
b_{i}\left(G_{1}\right) \geq b_{i}\left(G_{2}\right) \text { for all } i \geq 0 \Rightarrow E\left(G_{1}\right) \geq E\left(G_{2}\right) \tag{4}
\end{equation*}
$$

If $b_{i}\left(G_{1}\right) \geq b_{i}\left(G_{2}\right)$ holds for all $i \geq 0$, then we write $G_{1} \succeq G_{2}$ or $G_{2} \preceq G_{1}$. If $G_{1} \succeq G_{2}$ and there exists some $i_{0}$ such that $b_{i_{0}}\left(G_{1}\right)>b_{i_{0}}\left(G_{2}\right)$, then we write $G_{1} \succ G_{2}$.

According to the above relations, the following lemma follows readily.

Lemma 2. Let $G_{1}$ and $G_{2}$ be two graphs. Then $G_{1} \succeq G_{2}$ implies that $E\left(G_{1}\right) \geq E\left(G_{2}\right)$ and $G_{1} \succ G_{2}$ implies that $E\left(G_{1}\right)>E\left(G_{2}\right)$.

The following lemma is crucial to the proof of our main result.

Lemma 3. Let $G$ be a unicyclic graph on $n$ vertices with its cycle being $C_{l}$. Let uv be an edge in $E(G)$, we have
(a). If $u v \in C_{l}$, then $b_{i}(G)=b_{i}(G-u v)+b_{i-2}(G-u-v)-2 b_{i-l}\left(G-C_{l}\right)$ if $l \equiv 0(\bmod 4)$ and $b_{i}(G)=b_{i}(G-u v)+b_{i-2}(G-u-v)+2 b_{i-l}\left(G-C_{l}\right)$ if $l \not \equiv 0(\bmod 4)$;
(b). If $u v \notin C_{l}$, then $b_{i}(G)=b_{i}(G-u v)+b_{i-2}(G-u-v)$. In particular, if uv is a pendent edge with pendent vertex $v$, then $b_{i}(G)=b_{i}(G-v)+b_{i-2}(G-u-v)$.

Proof. Recall that

$$
\begin{equation*}
\phi(G ; x)=\phi(G-u v ; x)-\phi(G-u-v ; x)-2 \sum_{C \in \mathscr{C}_{u v}} \phi(G-C ; x), \tag{5}
\end{equation*}
$$

where $\mathscr{C}_{u v}$ denotes the set of cycles containing $u v$.
One can easily obtain the desired result by equating the coefficients of $x^{n-i}$ on both sides of Eq.(5).
F. Li and B. Zhou obtained the following result in [21].

Lemma 4. Let $G$ be a unicyclic graph in $\mathscr{U}_{n}$ and $G^{\prime}$ the graph obtained from $G$ by deleting at least one edge outside its unique cycle. Then $G^{\prime} \prec G$.
I. Gutman [3] show that $n$-vertex path $P_{n}$ is the unique graph with the maximal energy among all all acyclic graphs on $n$ vertices. The following lemma could be found in [1] as proposition 9.

Lemma 5. Let $T$ be a tree of order $n \geq 6$ not isomorphic to $P_{n}$. Then $E(T) \leq E\left(T_{n}^{2}\right)$ with equality if and only if $T \cong T_{n}^{2}$, where $T_{n}^{2}$ is the tree obtained by pasting one endpoint of $P_{n-4}$ to the middle vertex of $P_{5}$. (See Fig.2. for $T_{n}^{2}$ ).

In addition to the trees with maximal and second-maximal energy, also the trees with thirdmaximal, fourth-maximal, ... energy are determined by F. Zhang and H. Li [6].


$$
T_{n}^{2} \text { with } n \geq 8 \text { vertices. }
$$

## Fig.2.

Lemmas 6-8 given below are due to Y. Hou in [10].

Lemma 6. Let $G \in \mathscr{U}_{n}(l)$ with $l \not \equiv 0(\bmod 4)$. If $G \not \equiv P_{n}^{l}$, then $G \prec P_{n}^{l}$.

Let $\mathcal{C}(n, l)$ be the set of unicyclic graphs obtained from $C_{l}$ by attaching to it $n-l$ pendent vertices.

Lemma 7. Let $G \in \mathscr{U}_{n}(l)$ with $l \equiv 0(\bmod 4)$. If $G \not \equiv \mathcal{C}(n, l), P_{n}^{l}$, then $G \prec P_{n}^{l}$.

Lemma 8. Let $G$ be any connected graph in $\mathscr{U}_{n}$ and $G \nsupseteq C_{n}$. Then $E(G) \leq E\left(P_{n}^{6}\right)$ with equality only if $l=6$.

Lemma 9. Suppose $4 \leq l \leq n-6$. If $l \neq 4,6$, then $P_{l-2} \cup T_{n-l}^{2} \preceq P_{4} \cup T_{n-6}^{2} \preceq P_{2} \cup T_{n-4}^{2}$.

Proof. From [3], we know that $P_{2} \cup P_{n-2} \succeq P_{4} \cup P_{n-4} \succeq P_{i} \cup P_{n-i}$ for any integer $1 \leq i \leq n-1$ and $i \neq 2,4$. Note that

$$
\begin{aligned}
& m\left(P_{l-2} \cup T_{n-l}^{2} ; k\right)=m\left(P_{l-2} \cup P_{2} \cup P_{n-l-2} ; k\right)+m\left(P_{l-2} \cup P_{2} \cup P_{n-l-5} ; k-1\right), \\
& m\left(P_{4} \cup T_{n-6}^{2} ; k\right)=m\left(P_{4} \cup P_{2} \cup P_{n-8} ; k\right)+m\left(P_{4} \cup P_{2} \cup P_{n-11} ; k-1\right), \\
& m\left(P_{2} \cup T_{n-4}^{2} ; k\right)=m\left(P_{2} \cup P_{2} \cup P_{n-6} ; k\right)+m\left(P_{2} \cup P_{2} \cup P_{n-9} ; k-1\right) .
\end{aligned}
$$

Hence the result follows.

Lemma 10. Suppose $(i, j, k)$ is a 3 -element ordered pair with $1 \leq i \leq j \leq k$ and $i+j+k=n$. If $(i, j, k) \neq(2,2, n-4),(2,4, n-6)$, then $P_{i} \cup P_{j} \cup P_{k} \preceq P_{2} \cup P_{4} \cup P_{n-6} \preceq P_{2} \cup P_{2} \cup P_{n-4}$.

Proof. If $j \neq 2$, then

$$
\begin{aligned}
P_{i} \cup\left(P_{j} \cup P_{k}\right) & \preceq P_{i} \cup\left(P_{4} \cup P_{j+k-4}\right) \\
& =P_{4} \cup\left(P_{i} \cup P_{j+k-4}\right) \\
& \preceq P_{4} \cup\left(P_{2} \cup P_{i+j+k-6}\right)=P_{2} \cup\left(P_{4} \cup P_{n-6}\right) .
\end{aligned}
$$

Similarly, if $i \neq 2$, we can show that $P_{i} \cup P_{j} \cup P_{k} \preceq P_{2} \cup P_{4} \cup P_{n-6}$. Since $P_{2} \cup P_{4} \cup P_{n-6} \preceq$ $P_{2} \cup P_{2} \cup P_{n-4}$, then the result follows.

Theorem 11. Let $G \in \mathcal{B U}^{*}{ }_{n, 1}$ with $n \geq 8$ vertices. If $G \nsupseteq K_{n}^{6}$, then $G \prec K_{n}^{6}$.
Proof. Let $G$ be any graph in $\mathcal{B \mathcal { U } ^ { * }}{ }_{n, 1}$ and $C_{l}$ be the unique cycle in $G$. Since $G \not \equiv P_{n}^{l}, G$ has at least two pendent vertices. Let $v$ be the pendent vertex in $G$ such that $d_{G}\left(v, C_{l}\right)=1$ and $u$ its unique neighbor. Note that $G-v-u$ is a acyclic graph on $n-2$ vertices. So $G-v-u \preceq P_{n-2}$. Since $G-v \nsupseteq C_{n-1}$, then $G-v \preceq P_{n-1}^{6}$ by lemma 8. According to lemma 3(b), we get

$$
\begin{aligned}
b_{2 k}(G) & =b_{2 k}(G-v)+b_{2 k-2}(G-v-u) \\
& \leq b_{2 k}\left(P_{n-1}^{6}\right)+b_{2 k-2}\left(P_{n-2}\right) \\
& =b_{2 k}\left(K_{n}^{6}\right) .
\end{aligned}
$$

If $G \not \not K_{n}^{6}$, we can always find a positive integer $k_{0}$ such that $b_{2 k_{0}}(G)<b_{2 k_{0}}\left(K_{n}^{6}\right)$. This completes the proof.

Lemma 12. Let $G \in \mathcal{B} \mathcal{U}^{* b}{ }_{n, 2}(l)$ with $n=l+3$, then $G \preceq K_{n}^{l}$.

Proof. Obviously $G_{1}$ is the single element in $\mathcal{B} \mathcal{U}_{n, 2}^{* b}(l)$ (see Fig.3. for $G_{1}$ ). In view of lemma 3(b), we obtain

$$
\begin{aligned}
b_{2 k}\left(K_{l+3}^{l}\right)-b_{2 k}\left(G_{1}\right) & =b_{2 k-2}\left(P_{l+1}\right)-b_{2 k-2}\left(C_{l}\right) \\
& =m\left(P_{l+1} ; k-1\right)-m\left(P_{l} ; k-1\right)-m\left(P_{l-2} ; k-2\right) \pm 2
\end{aligned}
$$

where the last term " $\pm 2$ " should be erased if $2 k-2 \neq l$.
When $2 k-2 \neq l, b_{2 k}\left(K_{l+3}^{l}\right)-b_{2 k}\left(G_{1}\right)=m\left(P_{l-3} ; k-3\right) \geq 0$. When $2 k-2=l$ and $l \equiv 0(\bmod 4)$, we have $b_{2 k}\left(K_{l+3}^{l}\right)-b_{2 k}\left(G_{1}\right)=m\left(P_{l-3} ; k-3\right)+2>0$. When $2 k-2=l$ and $l \not \equiv 0(\bmod 4)$, we have $b_{2 k}\left(K_{l+3}^{l}\right)-b_{2 k}\left(G_{1}\right)=m\left(P_{l-3} ; k-3\right)-2=m\left(P_{l-3} ; \frac{l}{2}-2\right)-2 \geq 0$.

Consequently, the result follows.


Fig.3.

Lemma 13. Let $G \in \mathcal{B U}^{* b}{ }_{n, 2}(l)$ with $n=l+4$, then $G \preceq R_{n}^{l}$.

Proof. It's evident that $G$ must be one of graphs $G_{2}-G_{5}$ as shown in Fig.3.
According to lemmas 3(b) and 4, one can easily obtain that $G_{2} \succ G_{4}$. In the following, we will show that $R_{n}^{l} \succ G_{2}, G_{3}, G_{5}$. Apply lemma 3(b) once again, we obtain

$$
\begin{aligned}
b_{2 k}\left(R_{l+4}^{l}\right)-b_{2 k}\left(G_{2}\right)= & b_{2 k}\left(P_{l+2}^{l}\right)+b_{2 k-2}\left(P_{l+2}^{l}\right)+b_{2 k-2}\left(P_{l+1}\right)-b_{2 k}\left(P_{l+3}^{l}\right) \\
& -b_{2 k-2}\left(P_{2} \cup C_{l}\right) \\
= & b_{2 k-2}\left(P_{l+2}^{l}\right)+b_{2 k-2}\left(P_{l+1}\right)-b_{2 k-2}\left(P_{l+1}^{l}\right)-b_{2 k-2}\left(C_{l}\right) \\
& -b_{2 k-4}\left(C_{l}\right) \\
= & \cdots \\
= & b_{2 k-2}\left(P_{l+1}\right)-b_{2 k-2}\left(C_{l}\right) .
\end{aligned}
$$

Similar to the proof of lemma 12 , we can show that $G_{2} \preceq R_{l+4}^{l}$.
Similarly,

$$
\begin{aligned}
b_{2 k}\left(R_{l+4}^{l}\right)-b_{2 k}\left(G_{3}\right)= & b_{2 k}\left(P_{l+2}^{l}\right)+b_{2 k-2}\left(P_{l+2}^{l}\right)+b_{2 k-2}\left(P_{l+1}\right)-b_{2 k}\left(P_{l+3}^{l}\right) \\
& -b_{2 k-2}\left(P_{l+1}^{l}\right) \\
= & \cdots \\
= & b_{2 k-4}\left(C_{l}\right)+b_{2 k-2}\left(P_{l+1}\right)-b_{2 k-4}\left(P_{l-1}\right)-b_{2 k-2}\left(C_{l}\right) .
\end{aligned}
$$

If $2 k-4 \neq l$ and $2 k-2 \neq l$, then $b_{2 k}\left(R_{l+4}^{l}\right)-b_{2 k}\left(G_{3}\right)=m\left(P_{l-3} ; k-3\right)+2 m\left(P_{l-2} ; k-3\right) \geq 0$. If $2 k-4=l$ or $2 k-2=l$, then

$$
\begin{aligned}
b_{2 k}\left(R_{l+4}^{l}\right)-b_{2 k}\left(G_{3}\right) & \geq m\left(P_{l-3} ; k-3\right)+2 m\left(P_{l-2} ; k-3\right)-2 \\
& \geq\left\{\begin{array}{l}
2 m\left(P_{l-2} ; \frac{l}{2}-1\right)-2=0, \quad 2 k-4=l \\
2 m\left(P_{l-2} ; \frac{l}{2}-2\right)-2 \geq 0, \quad 2 k-2=l
\end{array}\right.
\end{aligned}
$$

Thus $G_{3} \preceq R_{l+4}^{l}$.

It is easy to obtain that $G_{5} \prec R_{l+4}^{l}$ by means of lemma 3 . This completes the proof.

Lemma 14. Let $n \geq 10$ and $4 \leq l \leq n-4$. If $l \neq 6$, then $R_{n}^{l} \prec R_{n}^{6}$.

Proof. By lemma 3(b), we have

$$
\begin{aligned}
b_{2 k}\left(R_{n}^{l}\right) & =b_{2 k}\left(K_{n-1}^{l}\right)+b_{2 k-2}\left(P_{n-2}^{l}\right) \\
& =b_{2 k}\left(P_{n-2}^{l}\right)+b_{2 k-2}\left(P_{n-2}^{l}\right)+b_{2 k-2}\left(P_{n-3}\right) \\
b_{2 k}\left(R_{n}^{6}\right) & =b_{2 k}\left(P_{n-2}^{6}\right)+b_{2 k-2}\left(P_{n-2}^{6}\right)+b_{2 k-2}\left(P_{n-3}\right)
\end{aligned}
$$

Since $n-2 \geq l+2$, the lemma follows as expected by lemma 8 .

By the same reasoning as employed in lemma 14, we can prove:

Lemma 15. Suppose $n \geq 8$ and $4 \leq l \leq n-2$. If $l \neq 6$, then $K_{n}^{l} \prec K_{n}^{6}$.

Lemma 16. For $n \geq 10$, we have $K_{n}^{6} \prec R_{n}^{6}$.


Fig. 4.
For $2 \leq i \leq n-l-1$ and $n-l \geq 5$, we use $M_{n}^{l, i}$ to denote the graph obtained by joining a vertex of $C_{l}$ by a new edge with the $i^{t h}$ vertex of path $P_{n-l}$, where the vertices of $P_{n-l}$ are labelled according to their natural orderings.

Theorem 17. Let $G \in \mathcal{B} \mathcal{U}^{* b}{ }_{n, 2}$ with $n \geq 13$. If $G \nsubseteq M_{n}^{n-5,2}, M_{n}^{n-5,3}, M_{n}^{6,3}$ and $Q_{n}^{6}$, then $G \prec M_{n}^{6,3}$ or $Q_{n}^{6}$.
 then $n \geq l+3$.

If $n=l+3$ or $l+4$, the result is evidently true from the combination of lemmas 12-16. So we may suppose that $n \geq l+5$ herein. We shall prove the theorem by distinguishing between two cases.

Case 1. $l=4$.
By means of lemmas 3(a) and 5, we have

$$
\begin{aligned}
b_{2 k}(G) & =m(G ; k)-2 b_{2 k-4}\left(G-C_{4}\right) \\
& \leq m(G ; k) \\
& \leq m\left(T_{n}^{2} ; k\right)+m\left(P_{2} \cup T_{n-4}^{2} ; k-1\right) \\
& =m\left(Q_{n}^{4} ; k\right) .
\end{aligned}
$$

In the following, we shall prove that $b_{2 k}\left(Q_{n}^{6}\right) \geq m\left(Q_{n}^{4} ; k\right)$ for all $k \geq 0$.
In view of lemma 3(a),

$$
b_{2 k}\left(Q_{n}^{6}\right)=m\left(T_{n}^{2} ; k\right)+m\left(P_{4} \cup T_{n-6}^{2} ; k-1\right)+2 m\left(T_{n-6}^{2} ; k-3\right) .
$$

Thus

$$
\begin{aligned}
b_{2 k}\left(Q_{n}^{6}\right)-m\left(Q_{n}^{4} ; k\right)= & m\left(P_{4} \cup T_{n-6}^{2} ; k-1\right)+2 m\left(T_{n-6}^{2} ; k-3\right)-m\left(P_{2} \cup T_{n-4}^{2} ; k-1\right) \\
= & m\left(P_{2} \cup P_{2} \cup T_{n-6}^{2} ; k-1\right)+m\left(T_{n-6}^{2} ; k-2\right)+2 m\left(T_{n-6}^{2} ; k-3\right) \\
& -m\left(P_{2} \cup P_{2} \cup T_{n-6}^{2} ; k-1\right)-m\left(P_{2} \cup T_{n-7}^{2} ; k-2\right) \\
= & m\left(T_{n-6}^{2} ; k-2\right)-m\left(T_{n-7}^{2} ; k-2\right)+2 m\left(T_{n-6}^{2} ; k-3\right)-m\left(T_{n-7}^{2} ; k-3\right) \\
\geq & 0 .
\end{aligned}
$$

So $b_{2 k}\left(Q_{n}^{6}\right) \geq b_{2 k}(G)$ and $b_{2 k}\left(Q_{n}^{6}\right) \geq b_{2 k}\left(Q_{n}^{4}\right)$ for all $k \geq 0$ in this case. In particular, $b_{6}\left(Q_{n}^{6}\right)>b_{6}(G)$ and $b_{6}\left(Q_{n}^{6}\right)>b_{6}\left(Q_{n}^{4}\right)$. Hence $G \prec Q_{n}^{6}$ and $Q_{n}^{4} \prec Q_{n}^{6}$.

Case 2. $l \geq 6$.
Case 2.1. $G \cong M_{n}^{l, i}$ for some $2 \leq i \leq n-l-1$. (See Fig.4. for $M_{n}^{l, i}$ )
In this case, we claim that $G \prec M_{n}^{6,3}$. Since $G \nsupseteq M_{n}^{n-5,2}\left(\cong M_{n}^{n-5,4}\right), M_{n}^{n-5,3}$, then $n-l \geq 6$.

Firstly, we prove that if $i \neq 3, n-l-2$, then $M_{n}^{l, i} \prec M_{n}^{l, 3}\left(\cong M_{n}^{l, n-l-2}\right)$.
Note that

$$
\begin{gathered}
b_{2 k}\left(M_{n}^{l, i}\right)=b_{2 k}\left(C_{l} \cup P_{n-l}\right)+b_{2 k-2}\left(P_{l-1} \cup P_{i-1} \cup P_{n-l-i}\right), \\
b_{2 k}\left(M_{n}^{l, 3}\right)=b_{2 k}\left(C_{l} \cup P_{n-l}\right)+b_{2 k-2}\left(P_{l-1} \cup P_{2} \cup P_{n-l-3}\right) .
\end{gathered}
$$

By means of lemma 10, it's not difficult to show that $P_{l-1} \cup P_{i-1} \cup P_{n-l-i} \prec P_{l-1} \cup P_{2} \cup P_{n-l-3}$. So there exists some $k_{0}$ such that $b_{2 k_{0}}\left(M_{n}^{l, 3}\right)>b_{2 k_{0}}\left(M_{n}^{l, i}\right)$ and then $M_{n}^{l, i} \prec M_{n}^{l, 3}$.

Secondly, we will demonstrate that if $l \neq 6$, i.e., $l \geq 8$, then $M_{n}^{l, 3} \prec M_{n}^{6,3}$.

By lemma 3(a), we deduce that

$$
\begin{aligned}
& b_{2 k}\left(M_{n}^{l, 3}\right)=b_{2 k}\left(T_{1}\right)+b_{2 k-2}\left(P_{l-2} \cup P_{n-l}\right) \pm 2 b_{2 k-l}\left(P_{n-l}\right), \\
& b_{2 k}\left(M_{n}^{6,3}\right)=b_{2 k}\left(T_{2}\right)+b_{2 k-2}\left(P_{4} \cup P_{n-6}\right)+2 b_{2 k-6}\left(P_{n-6}\right) .
\end{aligned}
$$

where $T_{1}\left(\right.$ resp. $\left.T_{2}\right)$ is the acyclic graph of order $n$ obtained from $M_{n}^{l, 3}$ (resp. $M_{n}^{6,3}$ ) by deleting one edge on $C_{l}$ (resp. $C_{6}$ ) incident with the unique 3-degree vertex of $C_{l}$ (resp. $C_{6}$ ).

Moreover,

$$
\begin{gathered}
b_{2 k}\left(T_{1}\right)=b_{2 k}\left(P_{2} \cup P_{n-2}\right)+b_{2 k-2}\left(P_{1} \cup P_{l} \cup P_{n-l-3}\right), \\
b_{2 k}\left(T_{2}\right)=b_{2 k}\left(P_{2} \cup P_{n-2}\right)+b_{2 k-2}\left(P_{1} \cup P_{6} \cup P_{n-9}\right) .
\end{gathered}
$$

Furthermore,

$$
\begin{aligned}
b_{2 k-6}\left(P_{n-6}\right)=m\left(P_{n-6} ; k-3\right) & =m\left(P_{n-7} ; k-3\right)+m\left(P_{n-8} ; k-4\right) \\
& \geq m\left(P_{n-8} ; k-4\right) \\
& \geq \cdots \\
& \geq m\left(P_{n-6-(l-6)} ; k-3-\frac{l-6}{2}\right) \\
& =m\left(P_{n-l} ; k-\frac{l}{2}\right)=b_{2 k-l}\left(P_{n-l}\right) .
\end{aligned}
$$

When $n-l \neq 7$, we clearly have $P_{1} \cup P_{l} \cup P_{n-l-3} \preceq P_{1} \cup P_{6} \cup P_{n-9}$ since $l \geq 8$. Thus $T_{1} \preceq T_{2}$ and then $M_{n}^{l, 3} \preceq M_{n}^{6,3}$.

When $n-l=7$,

$$
\begin{aligned}
b_{2 k}\left(M_{n}^{6,3}\right)-b_{2 k}\left(M_{n}^{l, 3}\right) \geq & b_{2 k-2}\left(P_{4} \cup P_{n-6}\right)-b_{2 k-2}\left(P_{7} \cup P_{n-9}\right)+b_{2 k-2}\left(P_{6} \cup P_{n-9}\right) \\
& -b_{2 k-2}\left(P_{4} \cup P_{n-7}\right) \\
= & m\left(P_{4} \cup P_{n-8} ; k-2\right)-m\left(P_{5} \cup P_{n-9} ; k-2\right) \geq 0 .
\end{aligned}
$$

So $M_{n}^{l, 3} \preceq M_{n}^{6,3}$.
Since $b_{0}\left(P_{n-6}\right)=1>0=b_{6-l}\left(P_{n-l}\right)$, then $b_{6}\left(M_{n}^{6,3}\right)>b_{6}\left(M_{n}^{l, 3}\right)$. This gives $M_{n}^{l, 3} \prec M_{n}^{6,3}$.
Case 2.2. $G \nsubseteq M_{n}^{l, i}$ for any $2 \leq i \leq n-l-1$.
Since $G \in \mathcal{B} \mathcal{U}^{* b}{ }_{n, 2}, C_{l}$ has exactly one branched vertex. Let $u$ be such a branched vertex and $w$ be one of its neighbors lying on $C_{l}$. By lemma 3(a),

$$
\begin{aligned}
b_{2 k}(G) & =b_{2 k}(G-u w)+b_{2 k-2}(G-u-w) \pm 2 b_{2 k-l}\left(G-C_{l}\right) \\
& \leq b_{2 k}\left(T_{n}^{2}\right)+b_{2 k-2}\left(P_{l-2} \cup T_{n-l}\right) \pm 2 b_{2 k-l}\left(T_{n-l}\right),
\end{aligned}
$$

where $T_{n-l}$ denotes the forest obtained by deleting the cycle $C_{l}$ from $G$. As $T_{n-l} \not \equiv P_{n-l}$ ( otherwise $G \cong P_{n}^{l}$ or $M_{n}^{l, i}$, a contradiction), we have $T_{n-l} \preceq T_{n-l}^{2}$ by lemma 5 . Because $l \geq 6$, we have $P_{l-2} \cup T_{n-l}^{2} \preceq P_{4} \cup T_{n-6}^{2}$ by lemma 9 .

When $l \equiv 0(\bmod 4)$, we have

$$
b_{2 k}(G) \leq b_{2 k}\left(T_{n}^{2}\right)+b_{2 k-2}\left(P_{4} \cup T_{n-6}^{2}\right)+2 b_{2 k-6}\left(T_{n-6}^{2}\right)=b_{2 k}\left(Q_{n}^{6}\right)
$$

Moreover, there exists some $k_{0}$ such that $b_{2 k_{0}}\left(Q_{n}^{6}\right)>b_{2 k_{0}}(G)$ since $G \not \equiv Q_{n}^{6}$.
When $l \not \equiv 0(\bmod 4)$, we have

$$
\begin{aligned}
m\left(T_{n-6}^{2} ; k-3\right) & =m\left(T_{n-7}^{2} ; k-3\right)+m\left(T_{n-8}^{2} ; k-4\right) \\
& \geq m\left(T_{n-8}^{2} ; k-4\right) \\
& \geq \cdots \\
& \geq m\left(T_{n-6-(l-6)}^{2} ; k-3-\frac{l-6}{2}\right) \\
& =m\left(T_{n-l}^{2} ; k-\frac{l}{2}\right) .
\end{aligned}
$$

Hence $b_{2 k}(G) \leq b_{2 k}\left(T_{n}^{2}\right)+b_{2 k-2}\left(P_{l-2} \cup T_{n-l}^{2}\right)+2 b_{2 k-l}\left(T_{n-l}^{2}\right) \leq b_{2 k}\left(T_{n}^{2}\right)+b_{2 k-2}\left(P_{4} \cup T_{n-6}^{2}\right)+$ $2 b_{2 k-6}\left(T_{n-6}^{2}\right)=b_{2 k}\left(Q_{n}^{6}\right)$. If $l \neq 6$, there must exist some $k_{0}^{\prime}$ such that $b_{2 k_{0}^{\prime}}\left(Q_{n}^{6}\right)>b_{2 k_{0}^{\prime}}(G)$.

From the combination of cases 1 and 2 it follows the present theorem as expected.

Lemma 18. Let $G \in \mathcal{B U}^{*}{ }_{n, 2}(l)$ with $n=l+4$ or $l+5$. If $G \not \nexists R_{n}^{l}$, then $G \prec R_{n}^{l}$.

Proof. We consider only the case that $n=l+4$. Since $G \in \mathcal{B} \mathcal{U}^{*}{ }_{n, 2}, G$ must have a pendent vertex $v$ such that $d_{G}\left(v, C_{l}\right)=2$ and $d_{G}(u)=2$, where $u$ is the unique neighbor of $v$. Note that $G-v \in \mathcal{B U}^{*}{ }_{n-1,1}$, one can easily verify that $G-v \preceq K_{n-1}^{l}$ by lemma 3(b). Similarly, we can demonstrate that $G-u-v \preceq P_{n-2}^{l}$ since $G-u-v \notin \mathcal{C}(n-2, l)$ and $G-u-v \not \equiv C_{n-2}$. By lemma 3(b),

$$
b_{2 k}(G)=b_{2 k}(G-v)+b_{2 k-2}(G-u-v) \leq b_{2 k}\left(K_{n-1}^{l}\right)+b_{2 k-2}\left(P_{n-2}^{l}\right)=b_{2 k}\left(R_{n}^{l}\right) .
$$

If $G \not \equiv R_{n}^{l}$, we can always find a positive integer $k_{0}$ such that $b_{2 k_{0}}\left(R_{n}^{l}\right)>b_{2 k_{0}}(G)$.
When $n=l+5$, the lemma can be proved by the same reasoning as used above. So the result follows.


Proof. Let $G$ be any graph in $\mathcal{B U}^{* a}{ }_{n, 2}$ and $C_{l}$ be the unique cycle in $G$. Since $G \in \mathcal{B} \mathcal{U}_{n, 2}^{* a}$, then $n \geq l+4$. We shall prove this lemma by induction on $n-l$. When $n-l=4$ or 5 , the lemma is immediate from lemma 18. Suppose that $n-l \geq 6$ and the lemma is true for graphs in $\mathcal{B U}^{* a}{ }_{n-1,2}$ or $\mathcal{B} \mathcal{U}^{* a}{ }_{n-2,2}$. Now, let $G$ be graph in $\mathcal{B U}^{*}{ }_{n, 2}$ with $n-l \geq 6$. There're two cases we should distinguish between.

Case 1. $d_{G}\left(v, C_{l}\right)=2$ for any $v \in V_{p}(G)$.

Let $S$ be the set of vertices adjacent to pendent vertices in $G$. If $d_{G}(u)=2$ for some vertex $u \in S$, then by the same method as used in proving lemma 18, we can show that $G \prec R_{n}^{l}$ (Here $G \not \equiv R_{n}^{l}$ ). Suppose that $d_{G}(u) \geq 3$ for all vertices $u$ in $S$. Let $u$ be any vertex in $S$ and $v$ be one pendent vertex adjacent to it. Then $G-v \in \mathcal{B} \mathcal{U}^{*}{ }_{n-1,2}$ and thus $G-v \prec R_{n-1}^{l}$ by induction assumption. Since $d_{G}(u) \geq 3$, all connected components not containing $C_{l}$ of $G-v-u$ must be isolated vertices. So by lemma $4, G-v-u \prec G^{\prime}$, where $G^{\prime}$ is the graph by attaching all isolated vertices of $G-v-u$ to any vertex of $C_{l}$. Evidently, $G^{\prime} \in \mathcal{B} \mathcal{U}^{*}{ }_{n-2,1}$ and it's not difficult to obtain that $G^{\prime} \prec K_{n-2}^{l}$. By lemmas 3(b) and (6), $K_{n-2}^{l} \prec R_{n-2}^{l}$ since $n-2 \geq l+4$ and $l \not \equiv 0(\bmod 4)$.

Therefore $G \prec R_{n}^{l}$.
Case 2 There exists some pendent vertex $v$ in $V_{p}(G)$ such that $d_{G}\left(v, C_{l}\right) \geq 3$.
Let $w \in V_{p}(G)$ be the pendent vertex in $G$ such that $d_{G}\left(w, C_{l}\right)=\max \left\{d_{G}\left(x, C_{l}\right) \mid x \in V_{p}(G)\right\}$. Obviously $G-w \in \mathcal{B} \mathcal{U}^{* a}{ }_{n-1,2}$ and thus $G-w \preceq R_{n-1}^{l}$ by induction assumption.

Let $u$ be the unique neighbor of $w$. If $G-w-u$ is connected, then $G-w-u \in$ $\mathcal{B} \mathcal{U}^{* a}{ }_{n-2,2}\left(d_{G}\left(w, C_{l}\right) \geq 4\right)$ or $\mathcal{B} \mathcal{U}^{*}{ }_{n-2,1}\left(d_{G}\left(w, C_{l}\right)=3\right)$.

If $G-w-u \in \mathcal{B U}^{*}{ }_{n-2,1}$, then $G-w-u \preceq K_{n-2}^{l} \prec R_{n-2}^{l}($ as $n-2 \geq l+4$ and $l \not \equiv 0(\bmod 4))$.
If $G-w-u \in \mathcal{B U}^{* a}{ }_{n-2,2}$, then $G-w-u \preceq R_{n-2}^{l}$ by induction hypothesis.
If $G-w-u$ is disconnected, then $G-w-u \prec G^{\prime \prime} \prec K_{n-2}^{l} \prec R_{n-2}^{l}$, where $G^{\prime \prime}$ is the graph by attaching all isolated vertices of $G-w-u$ to any vertex of $C_{l}$.

Combining cases 1 and 2 , the proof is completed.

Let $G$ be any graph in $\mathcal{U}_{n}$ and $C_{l}$ the unique cycle in $G$. Given that all vertices of the cycle $C_{l}$ are ordered successively as $v_{1}, v_{2}, \cdots, v_{l}$. For any $v_{i} \in V\left(C_{l}\right)$, let $T_{\left[v_{i}\right]}$ denote the connected component containing $v_{i}$ of $G-v_{i-1} v_{i}-v_{i} v_{i+1}$.

Lemma 20. Let $G \in \mathcal{B} \mathcal{U}_{n, 2}^{* a}(l)$ with $l \equiv 0(\bmod 4), 4 \leq l \leq n-4$ and $n \geq 12$. Then $G \prec Q_{n}^{6}$ or $R_{n}^{6}$.

Proof. Since $G \in \mathcal{B} \mathcal{U}^{* a}{ }_{n, 2}$, then $n \geq l+4$. We consider the following two cases.
Case 1. For some branched vertex $v_{i} \in V\left(C_{l}\right), n\left(T_{\left[v_{i}\right]}\right)=3$, where $n\left(T_{\left[v_{i}\right]}\right)$ is the order of $T_{\left[v_{i}\right]}$.

Since $G \in \mathcal{B U}_{n, 2}^{* a}(l)$, then $T\left[v_{i}\right] \cong P_{3}$ and $v_{i}$ is one end-point of $P_{3}$. Let the vertices of $T\left[v_{i}\right]\left(\right.$ or $\left.P_{3}\right)$ be ordered successively as $v_{i}, v_{i}^{\prime}, v_{i}^{\prime \prime}$ such that $d\left(v_{i}^{\prime}\right)=2$ and $d\left(v_{i}^{\prime \prime}\right)=1$. Then $G-v_{i}^{\prime \prime} \in \mathcal{B} \mathcal{U}^{*}{ }_{n-1,1}$ and thus $G-v_{i}^{\prime \prime} \preceq K_{n-1}^{l} \prec K_{n-1}^{6}$ by theorem 11. Moreover, $G-v_{i}^{\prime \prime}-v_{i}^{\prime} \prec$ $P_{n-2}^{6}$ by lemma 8 since $G-v_{i}^{\prime \prime}-v_{i}^{\prime} \not \not C_{n-2}$. So $G \prec R_{n}^{6}$ in this case.

Case 2. For each branched vertex $v_{i} \in V\left(C_{l}\right), n\left(T_{\left[v_{i}\right]}\right) \geq 4$.
Let $v_{t}$ be any branched vertex on $C_{l}$. We can always find one neighbor, say $v_{t}^{\prime}$, of $v_{t}\left(v_{t}^{\prime}\right.$ lies
on $C_{l}$ ) such that

$$
b_{2 k}\left(G-v_{t} v_{t}^{\prime}\right)+b_{2 k-2}\left(G-v_{t}-v_{t}^{\prime}\right) \leq b_{2 k}\left(T_{n}^{2}\right)+b_{2 k-2}\left(P_{4} \cup T_{n-6}^{2}\right)(\text { by lemmas } 5 \text { and } 9)
$$

or

$$
b_{2 k}\left(G-v_{t} v_{t}^{\prime}\right)+b_{2 k-2}\left(G-v_{t}-v_{t}^{\prime}\right) \leq b_{2 k}\left(P_{n}\right)+b_{2 k-2}\left(P_{2} \cup P_{4} \cup P_{n-8}\right)(\text { by lemma } 10) .
$$

So

$$
\begin{aligned}
b_{2 k}(G) & =b_{2 k}\left(G-v_{t} v_{t}^{\prime}\right)+b_{2 k-2}\left(G-v_{t}-v_{t}^{\prime}\right)-2 b_{2 k-l}\left(G-C_{l}\right) \\
& \leq b_{2 k}\left(T_{n}^{2}\right)+b_{2 k-2}\left(P_{4} \cup T_{n-6}^{2}\right)+2 b_{2 k-6}\left(T_{n-6}^{2}\right)=b_{2 k}\left(Q_{n}^{6}\right)
\end{aligned}
$$

or

$$
\begin{aligned}
b_{2 k}(G) & =b_{2 k}\left(G-v_{t} v_{t}^{\prime}\right)+b_{2 k-2}\left(G-v_{t}-v_{t}^{\prime}\right)-2 b_{2 k-l}\left(G-C_{l}\right) \\
& \leq b_{2 k}\left(P_{n}\right)+b_{2 k-2}\left(P_{2} \cup P_{4} \cup P_{n-8}\right)+2 b_{2 k-6}\left(P_{2} \cup P_{n-8}\right)=b_{2 k}\left(R_{n}^{6}\right) .
\end{aligned}
$$

In either cases, there exists some $k_{0}$ such that $b_{2 k_{0}}(G)<b_{2 k_{0}}\left(R_{n}^{6}\right)$ or $b_{2 k_{0}}(G)<b_{2 k_{0}}\left(Q_{n}^{6}\right)$. This proves the lemma.

Theorem 21. Let $G \in \mathcal{B} \mathcal{U}^{* a}{ }_{n, 2}$ with $n \geq 12$. Then $G \prec Q_{n}^{6}$ or $R_{n}^{6}$.
 theorem is true by lemma 20 . If $l \not \equiv 0(\bmod 4)$, then $G \preceq R_{n}^{l}$ by lemma 19 . Since $n \geq 12$, we can easily verify that $R_{n}^{l} \preceq R_{n}^{6}$ and the theorem follows as desired.

Lemma 22. For $n \geq 13$, we have $M_{n}^{n-5,2} \prec M_{n}^{n-5,3} \prec R_{n}^{6}$.

Proof. In full analogy with the proof of subcase 2.1 of theorem 17, we can obtain that $M_{n}^{n-5,2} \prec M_{n}^{n-5,3}$. In what follows we shall verify that $M_{n}^{n-5,3} \prec R_{n}^{6}$.

By means of lemma 3(a), we have

$$
\begin{aligned}
b_{2 k}\left(R_{n}^{6}\right)= & b_{2 k}\left(P_{n}\right)+b_{2 k-2}\left(P_{2} \cup P_{4} \cup P_{n-8}\right)+2 b_{2 k-6}\left(P_{2} \cup P_{n-8}\right) \\
= & b_{2 k}\left(P_{2} \cup P_{n-2}\right)+b_{2 k-2}\left(P_{1} \cup P_{n-3}\right)+b_{2 k-2}\left(P_{2} \cup P_{4} \cup P_{n-8}\right) \\
& +2 b_{2 k-6}\left(P_{n-8}\right)+2 b_{2 k-8}\left(P_{n-8}\right), \\
b_{2 k}\left(M_{n}^{n-5,3}\right)= & b_{2 k}\left(T_{n}^{2}\right)+b_{2 k-2}\left(P_{5} \cup P_{n-7}\right) \pm 2 b_{2 k-(n-5)}\left(P_{5}\right) \\
= & b_{2 k}\left(P_{2} \cup P_{n-2}\right)+b_{2 k-2}\left(P_{1} \cup P_{2} \cup P_{n-5}\right)+b_{2 k-2}\left(P_{5} \cup P_{n-7}\right) \\
& \pm 2 b_{2 k-(n-5)}\left(P_{5}\right) .
\end{aligned}
$$

So

$$
\begin{aligned}
b_{2 k}\left(R_{n}^{6}\right)-b_{2 k}\left(M_{n}^{n-5,3}\right)= & b_{2 k-4}\left(P_{1} \cup P_{1} \cup P_{n-6}\right)+b_{2 k-2}\left(P_{2} \cup P_{4} \cup P_{n-8}\right) \\
& -b_{2 k-2}\left(P_{2} \cup P_{3} \cup P_{n-7}\right)-b_{2 k-4}\left(P_{1} \cup P_{2} \cup P_{n-7}\right)+ \\
& 2 b_{2 k-6}\left(P_{n-8}\right)+2 b_{2 k-8}\left(P_{n-8}\right) \mp 2 b_{2 k-(n-5)}\left(P_{5}\right) \\
\geq \geq^{(\star)} \quad & b_{2 k-4}\left(P_{n-6}\right)-b_{2 k-4}\left(P_{n-7}\right)-b_{2 k-6}\left(P_{n-7}\right)+2 b_{2 k-6}\left(P_{n-8}\right) \\
& +2 b_{2 k-8}\left(P_{n-8}\right) \mp 2 b_{2 k-(n-5)}\left(P_{5}\right) \\
= & -b_{2 k-8}\left(P_{n-9}\right)+2 b_{2 k-6}\left(P_{n-8}\right)+2 b_{2 k-8}\left(P_{n-8}\right) \mp 2 b_{2 k-(n-5)}\left(P_{5}\right) \\
\geq & 2 b_{2 k-6}\left(P_{n-8}\right)+b_{2 k-8}\left(P_{n-8}\right) \mp 2 b_{2 k-(n-5)}\left(P_{5}\right) \\
\geq \geq & 0 .
\end{aligned}
$$

where the inequality ( $\star$ ) holds due to the fact that $P_{2} \cup P_{4} \cup P_{n-8} \succeq P_{2} \cup P_{3} \cup P_{n-7}$.
If $n$ is even, $b_{2 k-(n-5)}\left(P_{5}\right)=0$ and the inequality $(\bullet)$ is evidently true. Suppose that $n$ is odd. If $n-5 \equiv 0(\bmod 4)$, the inequality $(\bullet)$ holds clearly. If $n-5 \not \equiv 0(\bmod 4)$ and $2 k-(n-5) \geq 6$, the result is obvious. If $n-5 \not \equiv 0(\bmod 4)$ and $2 k-(n-5)=4, b_{2 k-6}\left(P_{n-8}\right)=$ 0 and $b_{2 k-8}\left(P_{n-8}\right)=b_{n-9}\left(P_{n-8}\right)=m\left(P_{n-8} ; \frac{n-9}{2}\right)=m\left(P_{n-9} ; \frac{n-9}{2}\right)+m\left(P_{n-10} ; \frac{n-9}{2}-1\right)=$ $1+m\left(P_{n-10} ; \frac{n-11}{2}\right) \geq 1+2=b_{2 k-(n-5)}\left(P_{5}\right)$. If $n-5 \not \equiv 0(\bmod 4)$ and $2 k-(n-5)=2$, then $b_{2 k-6}\left(P_{n-8}\right)=b_{n-9}\left(P_{n-8}\right)=m\left(P_{n-8} ; \frac{n-9}{2}\right)=\cdots=1+m\left(P_{n-10} ; \frac{n-11}{2}\right) \geq 1+2=3$ and $b_{2 k-8}\left(P_{n-8}\right)=b_{n-11}\left(P_{n-8}\right)=m\left(P_{n-8} ; \frac{n-11}{2}\right)=m\left(P_{n-9} ; \frac{n-11}{2}\right)+m\left(P_{n-10} ; \frac{n-13}{2}\right)>2$. Hence $2 b_{2 k-6}\left(P_{n-8}\right)+b_{2 k-8}\left(P_{n-8}\right) \mp 2 b_{2 k-(n-5)}\left(P_{5}\right)>2 \times 3+2-2 \times 4=0$. If $n-5 \not \equiv 0(\bmod 4)$ and $2 k-(n-5)=0$, the inequality $(\bullet)$ is immediate by the same method as used above.

From above arguments we conclude that $b_{2 k}\left(R_{n}^{6}\right) \geq b_{2 k}\left(M_{n}^{n-5,3}\right)$ and $b_{6}\left(R_{n}^{6}\right)>b_{6}\left(M_{n}^{n-5,3}\right)$, which proved the lemma.

Theorem 23. Let $G \in \mathcal{B U}^{*}{ }_{n}$ with $n \geq 13$. Then $M_{n}^{6,3}$ has the maximal energy among all graphs in $\mathcal{B} \mathcal{U}^{*}{ }_{n}$.

Proof. According to theorems 11, 17 and 21 and lemmas 16 and 22, we need only to prove that $M_{n}^{6,3} \succ R_{n}^{6}, Q_{n}^{6}$.

Using lemma 3 , we obtain

$$
\begin{gather*}
b_{2 k}\left(M_{n}^{6,3}\right)=b_{2 k}\left(P_{2} \cup P_{n-2}^{6}\right)+b_{2 k-2}\left(P_{1} \cup C_{6} \cup P_{n-9}\right),  \tag{6}\\
b_{2 k}\left(R_{n}^{6}\right)=b_{2 k}\left(P_{2} \cup P_{n-2}^{6}\right)+b_{2 k-2}\left(P_{1} \cup P_{n-3}\right),  \tag{7}\\
b_{2 k}\left(Q_{n}^{6}\right)=b_{2 k}\left(P_{2} \cup P_{n-2}^{6}\right)+b_{2 k-2}\left(P_{1} \cup P_{2} \cup P_{n-5}^{6}\right) . \tag{8}
\end{gather*}
$$

To prove that $M_{n}^{6,3} \succ R_{n}^{6}$, it's sufficient to prove that $C_{6} \cup P_{n-9} \succ P_{n-3}$ by Eqs.(6) and (7). In view of lemma 3 , we obtain

$$
b_{2 k}\left(C_{6} \cup P_{n-9}\right)=b_{2 k}\left(P_{6} \cup P_{n-9}\right)+b_{2 k-2}\left(P_{4} \cup P_{n-9}\right)+2 b_{2 k-6}\left(P_{n-9}\right),
$$

$$
b_{2 k}\left(P_{n-3}\right)=b_{2 k}\left(P_{6} \cup P_{n-9}\right)+b_{2 k-2}\left(P_{5} \cup P_{n-10}\right) .
$$

It's easy to see that $b_{6}\left(C_{6} \cup P_{n-9}\right)>b_{6}\left(P_{n-3}\right)$. Therefore $C_{6} \cup P_{n-9} \succ P_{n-3}$ and then $M_{n}^{6,3} \succ R_{n}^{6}$.

Next, we shall prove that $M_{n}^{6,3} \succ Q_{n}^{6}$. Combining Eqs.(6) and (8), we need only to prove that $C_{6} \cup P_{n-9} \succ P_{2} \cup P_{n-5}^{6}$. In view of lemma 3(b), we obtain

$$
\begin{aligned}
& b_{2 k}\left(C_{6} \cup P_{n-9}\right)=b_{2 k}\left(C_{6} \cup P_{2} \cup P_{n-11}\right)+b_{2 k-2}\left(C_{6} \cup P_{1} \cup P_{n-12}\right), \\
& b_{2 k}\left(P_{2} \cup P_{n-5}^{6}\right)=b_{2 k}\left(C_{6} \cup P_{2} \cup P_{n-11}\right)+b_{2 k-2}\left(P_{2} \cup P_{5} \cup P_{n-12}\right) .
\end{aligned}
$$

In what follows, we shall prove that $C_{6} \cup P_{1} \cup P_{n-12} \succ P_{2} \cup P_{5} \cup P_{n-12}$. Once again by lemma 3, we have

$$
\begin{aligned}
b_{2 k}\left(C_{6} \cup P_{1} \cup P_{n-12}\right)= & b_{2 k}\left(P_{6} \cup P_{1} \cup P_{n-12}\right)+b_{2 k-2}\left(P_{4} \cup P_{1} \cup P_{n-12}\right)+2 b_{2 k-6}\left(P_{1} \cup P_{n-12}\right) \\
= & b_{2 k}\left(P_{1} \cup P_{2} \cup P_{4} \cup P_{n-12}\right)+b_{2 k-2}\left(P_{1} \cup P_{1} \cup P_{3} \cup P_{n-12}\right)+ \\
& b_{2 k-2}\left(P_{1} \cup P_{2} \cup P_{2} \cup P_{n-12}\right)+b_{2 k-4}\left(P_{n-12}\right)+2 b_{2 k-6}\left(P_{n-12}\right), \\
b_{2 k}\left(P_{2} \cup P_{5} \cup P_{n-12}\right)= & b_{2 k}\left(P_{2} \cup P_{2} \cup P_{3} \cup P_{n-12}\right)+b_{2 k-2}\left(P_{2} \cup P_{1} \cup P_{2} \cup P_{n-12}\right) \\
= & b_{2 k}\left(P_{1} \cup P_{1} \cup P_{2} \cup P_{3} \cup P_{n-12}\right)+b_{2 k-2}\left(P_{2} \cup P_{3} \cup P_{n-12}\right)+ \\
& b_{2 k-2}\left(P_{1} \cup P_{2} \cup P_{2} \cup P_{n-12}\right) .
\end{aligned}
$$

Obviously, $P_{1} \cup P_{2} \cup P_{4} \cup P_{n-12} \succ P_{1} \cup P_{1} \cup P_{2} \cup P_{3} \cup P_{n-12}$. So $b_{2 k}\left(C_{6} \cup P_{1} \cup P_{n-12}\right)-b_{2 k}\left(P_{2} \cup\right.$ $P_{5} \cup P_{n-12}$ )

$$
\begin{aligned}
\geq & b_{2 k-2}\left(P_{1} \cup P_{1} \cup P_{3} \cup P_{n-12}\right)-b_{2 k-2}\left(P_{2} \cup P_{3} \cup P_{n-12}\right) \\
& +b_{2 k-4}\left(P_{n-12}\right)+2 b_{2 k-6}\left(P_{n-12}\right) \\
= & b_{2 k-2}\left(P_{3} \cup P_{n-12}\right)-b_{2 k-2}\left(P_{3} \cup P_{n-12}\right)-b_{2 k-4}\left(P_{3} \cup P_{n-12}\right) \\
& +b_{2 k-4}\left(P_{n-12}\right)+2 b_{2 k-6}\left(P_{n-12}\right) \\
= & \cdots=0 .
\end{aligned}
$$

It's evident that there exists some $k_{0}$ such that $b_{2 k_{0}}\left(C_{6} \cup P_{1} \cup P_{n-12}\right)>b_{2 k_{0}}\left(P_{2} \cup P_{5} \cup P_{n-12}\right)$. So $C_{6} \cup P_{1} \cup P_{n-12} \succ P_{2} \cup P_{5} \cup P_{n-12}$ and then $C_{6} \cup P_{n-9} \succ P_{2} \cup P_{n-5}^{6}$. This completes the proof.

Acknowledgement The author is indebted to Professor Ivan Gutman for providing many helpful suggestions and pointing out an error, which improved greatly the previous version of this paper.

## References

[1] I. Gutman, Acyclic systems with extremal Huckel $\pi$ - electron energy, Theor. Chim. Acta. 45 (1977) 79-87.
[2] I. Gutman, Total $\pi$ - electron energy of benzenoid hydrocarbon, Topic. Curr. Chem. 162 (1992) 29-63.
[3] I. Gutman and O. E. Polansky, Mathematical Concepts in Organic Chemistry (Springer, Berlin, 1986).
[4] I. Gutman, Acyclic conjugated molecules, trees and their energies, J.Math. Chem. 2 (1987) 123-143.
[5] F. Zhang and H. Li, On acyclic conjugated molocules with minimal energies, Discrete Appl. Math. 92 (1999) 71-84.
[6] F. Zhang and H. Li, On maximal energy ordering of conjugated acyclic molecules, in: P.Hansen, P. Fowler, M. Zheng, Discrete Math. Chem., Am. Math. Soc., Providence, 2000, pp. 385-392.
[7] I. Gutman, Y. Hou, Bipartite unicyclic graphs with greatest energy MATCH Commun. Math. Comput. Chem. 43 (2001) 17-28.
[8] Y. Hou, Unicyclic graphs with minimal energy , J.Math.Chem. 3 (2001) 163-168.
[9] Y. Hou, Bicyclic graphs with minimal energy, Linear and Multilinear Algebra. 49 (2001) 347-354.
[10] Y. Hou, I. Gutman and C-H. Woo, Unicyclic graphs with maximal energy, Linear Algebra Appl. 356 (2002) 27-36.
[11] J. Rada and A. Tineo, Polygonal chains with minimal energy, Linear Algebra Appl. 372 (2003) 333-344.
[12] W. Yan, On the minimal energy of trees with a given diameter, Appl. Math . Lett. 18 (2005) 1046-1052.
[13] A. Yu, M. Lu, F. Tian, New upper bounds for the energy of graphs, MATCH Commun. Math. Comput. Chem. 53 (2005) 441-448.
[14] W. Yan, L. Ye, On the maximal energy and the Hosoya index of a type of trees with many pendant vertices, MATCH Commun. Math. Comput. Chem. 53 (2005) 449-459 .
[15] W. Lin, X. Guo, H. Li, On the extremal energies of trees with a given maximum degree, MATCH Commun. Math. Comput. Chem. 54 (2005) 363-378.
[16] F. Li, B. Zhou, Minimal energy of bipartite unicyclic graphs of a given bipartition , MATCH Commun. Math. Comput. Chem. 54 (2005) 379-388.
[17] G. Indulal, A. Vijayakumar, On a pair of equienergetic graphs, MATCH Commun. Math. Comput. Chem. 55 (2006) 83-90 .
[18] B. Zhou, Lower bounds for energy of quadrangle-free graphs, MATCH Commun. Math. Comput. Chem. 55 (2006) 91-94 .
[19] A. Chen, A. Chang, W. C. Shiu, Energy ordering of unicyclic graphs, MATCH Commun. Math. Comput. Chem. 55 (2006) 95-102.
[20] J. A. de la Peña, L. Mendoza, Moments and $\pi$-electron energy of hexagonal systems in 3-Space, Math.Comput. Chem. 56 (2006) 113-129.
[21] F. Li, B. Zhou, Minimal energy of unicyclic graphs of a given diameter, J.Math.Chem. (2006) Accepted.
[22] H. Hua, On minimal energy of unicyclic graphs with prescribed girth and pendent vertices, MATCH Commun. Math. Comput. Chem. 57 (2007) 351-361.
[23] I. Gutman, The energy of a graph:old and new results, in: Algebra Combinatorics and Applications eds. A.Betten, A.Kohnert, R.Laue and A.Wassermann(Springer -Verlag, Berlin,2001), pp.196-211.
[24] I. Gutman, Topology and stability of conjugated hydrocarbons. The dependence of total $\pi$-electron energy on molecular topology, J. Serb. Chem. Soc. 70 (2005) 441-456.
[25] D. Cvetkovic, M. Doob and H. Sachs, Spectra of Graphs, (Academic Press, New York, 1980).

