Ordering of Unicyclic Graphs with Perfect Matchings by Minimal Energies

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Abstract

The ordering of unicyclic graphs with perfect matchings having \(2n\) vertices according to their minimal energies is considered. Using the method of coefficient comparison and the theorem of zero points, we derive the first 7, 8, 7, 6, and 5 unicyclic graphs with perfect matchings for \(n \geq 45\), \(44 \geq n \geq 10\), \(9 \geq n \geq 8\), \(7 \geq n \geq 6\), and \(n = 5\), respectively.

1 Introduction

As pointed out by Gutman and Polansky [1], the total energy of all \(\pi\)-electrons in conjugated molecules, within the framework of Hückel molecular orbital (HMO) approximation, is a bridge between the chemical structure and its thermodynamic stability. The larger is the value of the energy, the greater is the thermodynamic stability of the corresponding compound [1]. Motivated by this reason, a number of results have been reached for the ordering of graphs with extremal energies, which is of practical importance and theoretical interest in the subject of chemical graph theory. For example, acyclic [2–8], unicyclic [9–15], bicyclic [16–18], tricyclic [19,20] graphs, and various chains [21–23] were considered.
Let $G$ be a graph with $n$ vertices and $A(G)$ its adjacent matrix. The characteristic polynomial of $G$ is [24]

$$\phi(G, x) = \det[xI - A(G)] = \sum_{i=0}^{n} a_i x^{n-i} \quad (1)$$

where $I$ is the unit matrix of order $n$ and $a_0, a_1, \ldots, a_n$ are the coefficients of the characteristic polynomial of $G$. The $n$ roots of $\phi(G, x) = 0$ are denoted by $\lambda_1, \ldots, \lambda_n$, which are the eigenvalues of the corresponding graph $G$.

The total energy of all $\pi$-electrons in conjugated hydrocarbons, within the framework of HMO approximation [1, 24], can be reduced to

$$E(G) = \sum_{i=1}^{n} |\lambda_i| \quad (2)$$

$E(G)$ can also be expressed as the Coulson integral formula [1]

$$E(G) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{x^2} \ln \left[ \left( \sum_{j=0}^{[n/2]} b_{2j} x^{2j} \right)^2 + \left( \sum_{j=0}^{[n/2]} b_{2j+1} x^{2j+1} \right)^2 \right] \, dx \quad (3)$$

where $b_i(G) = |a_i(G)|$. Note that $b_0(G) = 1$, $b_1(G) = 0$ and $b_2(G)$ equals the number of edges in $G$. It can be seen from (3) that $E(G)$ is a strictly monotonously increasing function of $b_i(G)$. Let $G_1$ and $G_2$ be two unicyclic graphs, then

$$b_i(G_1) \geq b_i(G_2) \Rightarrow E(G_1) \geq E(G_2) \quad (4)$$

where $E(G_1) = E(G_2)$ if and only if (iff) $b_i(G_1) = b_i(G_2)$ for all $i \geq 0$ [9]. The relation (4) has been used in the study of energy and will be referred to as the method of coefficient comparison. For the sake of conciseness, we introduce the symbols “$\nrightarrow$”, “$\equiv$” and “$\Rightarrow$” as follows.

$$E(G_1) < E(G_2) \iff G_1 \nrightarrow G_2 \quad , \quad E(G_1) = E(G_2) \iff G_1 \equiv G_2$$

$$E(G_1) \leq E(G_2) \iff G_1 \Rightarrow G_2 \quad . \quad (5)$$

We denote by $\mathcal{K}_{2n}^l$ the set of unicyclic graphs with perfect matchings having $2n$ vertices, where $l$ is the length of the cycle contained in the graph. Some preliminary results for the minimal energy in $\mathcal{K}_{2n}^l$ have been reported. Wang et al. [11] obtained the graph with minimal energy for $n \geq 3$ and Li et al. [12] obtained the graphs with
the first and second minimal energies for \( n \geq 5 \). The further ordering of unicyclic graphs with perfect matchings by their minimal energies for \( n \geq 5 \) remains a task. In this paper, using the method of coefficient comparison in (4) and the theorem of zero points, we extend those results obtained by Wang et al. \[11\] and Li et al. \[12\]. We derive the first 7, 8, 7, 6, and 5 unicyclic graphs with perfect matchings for \( n \geq 45 \), \( 44 \geq n \geq 10 \), \( 9 \geq n \geq 8 \), \( 7 \geq n \geq 6 \), and \( n = 5 \), respectively.

2 Preliminaries

Let \( G \in \mathcal{K}_{2n}^l \) and \( m(G,k) \) be the number of \( k \)-matchings in \( G \), where \( 0 \leq k \leq n \). Obviously, \( m(G,1) = 2n \). In addition, it is consistent to define \( m(G,0) = 1 \). Let \( \hat{G} = G - M(G) - S_0 \), where \( M(G) \) is a perfect matching of \( G \) and \( S_0 \) is the set of isolated vertices in \( G - M(G) \). It is clear that \( |M(G)| = n \), where \( |M(G)| \) is the number of edges in \( M(G) \). We call \( \hat{G} \) the capped graph of \( G \) and \( G \) the original graph of \( \hat{G} \). Each \( k \)-matching \( \Omega \) of \( G \) can be partitioned into two parts: \( \Omega = \Phi \cup \Psi \), where \( \Phi \) is a matching in \( \hat{G} \) and \( \Psi \subset M(G) \).

Thus, we have \[3\]

\[
m(G,k) = \sum_{i=0}^{k} m(\hat{G},i) \left( \begin{array}{c} n-j \\ k-i \end{array} \right) = p + \sum_{i=2}^{k} m(\hat{G},i) \left( \begin{array}{c} n-j \\ k-i \end{array} \right)
\]

(6)

where

\[
p = \left( \begin{array}{c} n \\ k \end{array} \right) + n \left( \begin{array}{c} n-2 \\ k-1 \end{array} \right)
\]

and \( j \) is the number of edges in \( M(G) \) which are adjacent to the \( i \)-matching \( \Phi \).

In order to formulate our results, we simply quote some definitions for certain types of graphs and necessary lemmas.

For \( n \geq 3 \), \( P_n \) is a path with \( n \) vertices, and the vertices of \( P_n \) are labelled consecutively by \( v_1, v_2, \ldots, v_n \).

For \( l \geq 3 \), \( C_l \) is a cycle with \( l \) vertices, and the vertices of \( C_l \) are labelled consecutively by \( u_1, u_2, \ldots, u_l \).

For \( n \geq 3 \), \( X_n \) is the star \( K_{1,n-1} \).

For \( n \geq 5 \), \( Y_n \) is the graph obtained from \( P_4 \) by attaching \( n - 4 \) pendant edges to \( v_2 \).
For \( n \geq 5 \), \( Z_n \) is the graph obtained from \( P_4 \) by attaching \( n - 5 \) and one pendant edges to \( v_2 \) and \( v_3 \), respectively.

For \( n \geq 5 \), \( W_n \) is the graph obtained from \( P_5 \) by attaching \( n - 5 \) pendant edges to \( v_2 \).

**Lemma 1.** [1] Let \( e = uv \) be an edge of \( G \). If the edge \( e \) does not belong to any cycle, then

\[
\phi(G) = \phi(G - e) - \phi(G - u - v) .
\]

**Lemma 2.** [1] Let \( e = uv \) be an edge of \( G \). Then we have

\[
m(G, k) = m(G - e, k) + m(G - u - v, k - 1) .
\]

**Lemma 3.** [9,11] Let \( G \in K^l_{2n} \) and \( r \) be an integer with \( r \geq 1 \). Then

\[
b_{2k}(G) = \begin{cases} 
m(G, k) + 2(-1)^{r+1}m(G - C_l, k - r) & (l = 2r) \\
m(G, k) & (l = 2r + 1) \end{cases}
\]

\[
b_{2k+1}(G) = \begin{cases} 
0, & (l = 2r, l = 2r + 1 \& 2k + 1 < l) \\
2m(G - C_l, k - r) & (l = 2r + 1 \& 2k + 1 \geq l) \end{cases}
\]

**Lemma 4.** [2] Let \( T \) be a tree with \( n \) vertices, where \( n \geq 5 \). Then \( m(X_n, k) \leq m(Y_n, k) \leq m(Z_n, k) \leq m(W_n, k) \leq m(T, k) \), and the equalities do not hold for all \( k \), where \( T \neq X_n, Y_n, Z_n, W_n \) and \( 0 \leq k \leq \lceil n/2 \rceil \).

### 3 Main results

To obtain the main results of the present paper, we need to define some new graphs and deduce new results in Lemmas 5–11 firstly.

Let \( S^3_{2n} \) be the graph obtained from \( C_3 \) by attaching one pendant edge and \( n - 2 \) paths of length 2 to \( u_1 \).

Let \( R^3_{2n} \) be the graph obtained from \( C_3 \) by attaching one pendant edge to every vertex of \( C_3 \) and then by attaching \( n - 3 \) paths of length 2 to \( u_1 \).

Let \( Y^3_{2n} \) be the graph obtained from \( C_3 \) by attaching a path of length 2 to \( u_1 \) and then by attaching one pendant edge and \( n - 3 \) paths of length 2 to \( u_2 \).
Let $J^3_{2n}$ be the graph obtained from $C_3$ by attaching one pendant edge to $u_1$ and then by attaching $n - 2$ paths of length 2 to $u_2$.

Let $S^4_{2n}$ be the graph obtained from $C_4$ by attaching one pendant edge to $u_1$ and then by attaching one pendant edge and $n - 3$ paths of length 2 to $u_2$.

Let $Q^4_{2n}$ be the graph obtained from $C_4$ by attaching $n - 2$ paths of length 2 to $u_1$.

Let $R^4_{2n}$ be the graph obtained from $C_4$ by attaching one pendant edge to every vertex of $C_4$ and then by attaching $n - 4$ paths of length 2 to $u_1$.

Let $W^4_{2n}$ be the graph obtained from $C_4$ by attaching a path $P_3$ to $u_1$ of $C_4$ and then by attaching $n - 3$ paths of length 2 to the second vertex of $P_3$.

Let $Q^5_{2n}$ be the graph obtained from $C_5$ by attaching one pendant and $n - 3$ paths of length 2 to $u_1$.

For example, $S^3_8$, $R^3_8$, $Y^3_8$, $J^3_8$, $S^4_8$, $Q^4_8$, $R^4_8$, $W^4_8$, and $Q^5_8$ are shown in Fig. 1.

**Lemma 5.** $S^3_{2n} \rightarrow S^4_{2n}$ for $n \geq 7$ and $S^4_{2n} \rightarrow S^3_{2n}$ for $6 \geq n \geq 3$. 
Proof. Straightforward derivation by Lemma 1 yields

\[ \phi(S^3_{2n}, x) = (x^2 - 1)^{n-2} \left[ 1 - 2x - (2 + n)x^2 + x^4 \right] \]
\[ \triangleq (x^2 - 1)^{n-2} f_1(x) \]  
\[ \phi(S^4_{2n}, x) = (x^2 - 1)^{n-4} \left[ 1 - (3 + n)x^2 + (2 + 3n)x^4 - (4 + n)x^6 + x^8 \right] \]
\[ \triangleq (x^2 - 1)^{n-4} f_2(x) . \]

It is noted that the exact roots of \( f_1(x) = 0 \) and \( f_2(x) = 0 \) with respect to \( x \) can be obtained. However, it is too complex to compare the exact representations for the energies of \( S^3_{2n} \) and \( S^4_{2n} \) for an arbitrary \( n \). Therefore, approximate roots of \( f_1(x) = 0 \) and \( f_2(x) = 0 \) can be used instead. Suppose that the continuous function \( f_1(x) \) satisfies \( f_1(a) f_1(b) < 0 \) on a closed interval \([a, b]\). Then, according to the intermediate-value theorem [25], there exists a real number \( c \) in such a way that \( f_1(c) = 0 \) with \( a < c < b \). This property is referred to as the theorem of zero points hereinafter. Next it is necessary to identify \( a \) and \( b \) for every root \( x_i \) of \( f_1(x) = 0 \) to meet the requirement of \( f_1(a) f_1(b) < 0 \), where \( 1 \leq i \leq 4 \).

Obviously, we have

\[
\begin{align*}
  f_1(-\sqrt{n+2}) &= 1 + 2\sqrt{n+2} > 0 & (n \geq 3) \\
  f_1(-\sqrt{n+1}) &= -n + 2\sqrt{n+1} < 0 & (n \geq 5) \\
  f_1(-0.01) &= 1.0198 - 0.0001n < 0 & (n \geq 10199) \\
  f_1(-1/n) &= 1 + 1/n^4 - 2/n^2 + 1/n > 0 & (n \geq 3) \\
  f_1(1/n) &= 1 + 1/n^4 - 2/n^2 - 3/n > 0 & (n \geq 4) \\
  f_1(0.01) &= 0.9798 - 0.0001n < 0 & (n \geq 9798) \\
  f_1(\sqrt{n+1}) &= -n - 2\sqrt{1+n} < 0 & (n \geq 3) \\
  f_1(\sqrt{n+3}) &= 4 + n - 2\sqrt{3+n} > 0 & (n \geq 3). \\
\end{align*}
\]

According to the theorem of zero points, we have

\[
E(S^3_{2n}) = 2(n - 2) + \sum_{i=1}^{4} |x_i| < 2(n - 2) + \sqrt{n+2} + 0.01 + 0.01 + \sqrt{n+3}, \quad (n \geq 10199). \]  

(11)
The explicit expressions for $f_j(\cdot)$ with $j \geq 2$ can be obtained by a straightforward calculation and will be omitted hereinafter for the sake of conciseness. One can readily obtain the following expressions: $f_2(\sqrt{1/n}) > 0$ for $n \geq 4$, $f_2(\sqrt{2/n}) < 0$ for $n \geq 5$, $f_2(\sqrt{0.38}) < 0$ for $n \geq 3$, $f_2(\sqrt{0.39}) > 0$ for $n \geq 12$, $f_2(\sqrt{2.61}) > 0$ for $n \geq 384$, $f_2(\sqrt{2.62}) < 0$ for $n \geq 3$, $f_2(\sqrt{n}) < 0$ for $n \geq 3$ and $f_2(\sqrt{n+1.1}) > 0$ for $n \geq 23$. According to the theorem of zero points, we have

$$2(n - 4) + 2(\sqrt{1/n} + \sqrt{0.38} + \sqrt{2.61} + \sqrt{n}) < E(S_{2n}^4), \quad (n \geq 384). \quad (12)$$

It follows from $2(n - 2) + \sqrt{n} + 2 + 0.01 + 0.01 + \sqrt{n} + 3 < 2(n - 4) + 2(\sqrt{1/n} + \sqrt{0.38} + \sqrt{2.61} + \sqrt{n})$ that the right-hand side (RHS) of (11) is less than the left-hand side (LHS) of (12) as $n \geq 10199$. Therefore, $S_{2n}^3 \rightarrow S_{2n}^4$ for $n \geq 10199$. The calculation yields $S_{2n}^3 \rightarrow S_{2n}^4$ for $10198 \geq n \geq 7$ while $S_{2n}^4 \rightarrow S_{2n}^3$ for $6 \geq n \geq 3$. ■

**Lemma 6.** $S_{2n}^4 \rightarrow R_{2n}^3 \rightarrow Y_{2n}^3$ for $n \geq 4$.

**Proof.** Let $n \geq 4$. Wang et al. [11] obtained

$$b_{2k}(S_{2n}^4) = p - \left( \frac{n - 3}{k - 2} \right) + (n - 3) \left( \frac{n - 4}{k - 2} \right). \quad (13)$$

It is noted that $m(R_{2n}^3, 2) = n - 3$. Since each 2-matching of $R_{2n}^3$ are adjacent to four edges of $M(R_{2n}^3)$ and $m(R_{2n}^3, i) = 0$ for $3 \leq i \leq n$, from Lemma 3, we have

$$b_{2k}(R_{2n}^3) = m(R_{2n}^3, k) = p + (n - 3) \left( \frac{n - 4}{k - 2} \right). \quad (14)$$

From Lemma 3 and the fact that $R_{2n}^3 - C_3$ is composed of $n - 3$ independent edges and three isolated vertices, we obtain

$$b_{2k+1}(R_{2n}^3) = \begin{cases} 0 & (2k + 1 < 3) \\ 2 \left( \frac{n - 3}{k - 1} \right) & (2k + 1 \geq 3). \end{cases} \quad (15)$$

It is noted that $m(Y_{2n}^3, 2) = m(Y_{n+1}^3, 2) = n - 2$. Since one 2-matching of $Y_{2n}^3$ are adjacent to three edges of $M(Y_{2n}^3)$ and the other 2-matchings of $Y_{2n}^3$ to four edges of $M(Y_{2n}^3)$, and $m(Y_{2n}^3, i) = 0$ for $3 \leq i \leq n$, from Lemma 3, we have

$$b_{2k}(Y_{2n}^3) = m(Y_{2n}^3, k) = p + \left( \frac{n - 3}{k - 2} \right) + (n - 3) \left( \frac{n - 4}{k - 2} \right). \quad (16)$$
From Lemma 3 and the fact that $Y_{2n}^3 - C_3$ is composed of $n - 2$ independent edges and one isolated vertex, we obtain

$$b_{2k+1}(Y_{2n}^3) = \begin{cases} 0 & (2k + 1 < 3) \\ 2 \left( \frac{n-2}{k-1} \right) & (2k + 1 \geq 3) \end{cases}. \quad (17)$$

From (13), (14) and (16), we have $b_{2k}(S_{2n}^4) \leq b_{2k}(R_{2n}^3) \leq b_{2k}(Y_{2n}^3)$, where the equalities do not hold for all $k$. For example, $b_4(S_{2n}^4) < b_4(R_{2n}^3) < b_4(Y_{2n}^3)$. By Lemma 3, we have $b_{2k+1}(S_{2n}^4) = 0$. Therefore, by (15) and (17), we have $b_{2k+1}(S_{2n}^4) \leq b_{2k+1}(R_{2n}^3) \leq b_{2k+1}(Y_{2n}^3)$, where the equalities do not hold for all $k$. For example, $b_5(S_{2n}^4) = 0 < b_5(R_{2n}^3) < b_5(Y_{2n}^3)$. Thus, Lemma 6 holds. ■

**Lemma 7.** (i) $Y_{2n}^3 \to Q_{2n}^4$ for $n \geq 37$ and $Q_{2n}^4 \to Y_{2n}^3$ for $36 \geq n \geq 3$.

(ii) $Q_{2n}^5 \to Q_{2n}^4$ for $n \geq 40$ and $Q_{2n}^4 \to Q_{2n}^5$ for $39 \geq n \geq 3$.

**Proof.** Straightforward derivation by Lemma 1 yields

$$\phi(Y_{2n}^3, x) = (x^2 - 1)^{n-4} \left[ 1 - 2x - (5 + n)x^2 + 4x^3 + (4 + 3n)x^4 - 2x^5 - (4 + n)x^6 + x^8 \right]$$

$$\triangleq (x^2 - 1)^{n-4} f_3(x) \quad (18)$$

$$\phi(Q_{2n}^4, x) = x^2(x^2 - 1)^{n-3} \left[ 2n - (3 + n)x^2 + x^4 \right]$$

$$\triangleq x^2(x^2 - 1)^{n-3} f_4(x) \quad (19)$$

$$\phi(Q_{2n}^5, x) = (x^2 - 1)^{n-4} \left[ 1 + 2x - (6 + n)x^2 - 2x^3 + (5 + 3n)x^4 - (4 + n)x^6 + x^8 \right]$$

$$\triangleq (x^2 - 1)^{n-4} f_5(x). \quad (20)$$

Since $f_3(-\sqrt{n+1}) > 0$ for $n \geq 3$, $f_3(-\sqrt{n}) < 0$ for $n \geq 5$, $f_3(-1.61804) < 0$ for $n \geq 3$, $f_3(-1.61803) > 0$ for $n \geq 13237$, $f_3(-0.61806) > 0$ for $n \geq 2035$, $f_3(-0.61803) < 0$ for $n \geq 3$, $f_3(-0.01) < 0$ for $n \geq 10199$, $f_3(-1/n) > 0$ for $n \geq 3$, $f_3(1/n) > 0$ for $n \geq 3$, $f_3(0.01) < 0$ for $n \geq 9798$, $f_3(0.61802) < 0$ for $n \geq 3$, $f_3(0.61806) > 0$ for $n \geq 36416$, $f_3(1.61802) > 0$ for $n \geq 67715$, $f_3(1.61804) < 0$ for $n \geq 3$, $f_3(\sqrt{n}) < 0$ for $n \geq 3$, and $f_3(\sqrt{n+2}) > 0$ for $n \geq 6$, we have

$$E(Y_{2n}^3) < 2(n-4) + \sqrt{n+1} + 2(1.61804 + 0.61806 + 0.01)$$

$$+ \sqrt{n+2} \quad (n \geq 67715). \quad (21)$$
Since \( f_4(\sqrt{1.99}) > 0 \) for \( n \geq 201 \), \( f_4(\sqrt{2}) < 0 \) for \( n \geq 3 \), \( f_4(\sqrt{n + 0.5}) < 0 \) for \( n \geq 3 \), and \( f_4(\sqrt{n + 1.12}) > 0 \) for \( n \geq 18 \), we have

\[
2(n - 3) + 2(\sqrt{1.99} + \sqrt{n + 0.5}) < E(Q^4_{2n}) \quad (n \geq 201) . \quad (22)
\]

It follows from \( 2(n - 4) + \sqrt{n + 1} + 2(1.61804 + 0.61806 + 0.01) + \sqrt{n + 2} < 2(n - 3) + 2(\sqrt{1.99} + \sqrt{n + 0.5}) \) that the RHS of (21) is less than the LHS of (22) as \( n \geq 67715 \). Therefore, \( Y_2^3 \to Q_2^4 \) for \( n \geq 67715 \). The calculation yields \( Y_2^3 \to Q_2^4 \) for \( 67714 \geq n \geq 37 \) while \( Q_2^4 \to Y_2^3 \) for \( 36 \geq n \geq 3 \). Therefore Lemma 7(i) holds.

Since \( f_5(-\sqrt{n + 1}) > 0 \) for \( n \geq 3 \), \( f_5(-\sqrt{n}) < 0 \) for \( n \geq 3 \), \( f_5(-1.61803) > 0 \) for \( n \geq 3 \), \( f_5(-0.61806) < 0 \) for \( n \geq 3 \), \( f_5(-0.01) < 0 \) for \( n \geq 3 \), \( f_5(1/n) > 0 \) for \( n \geq 3 \), \( f_5(0.01) < 0 \) for \( n \geq 3 \), \( f_5(0.61802) < 0 \) for \( n \geq 5 \), \( f_5(0.61806) > 0 \) for \( n \geq 5 \), \( f_5(1.61803) > 0 \) for \( n \geq 138589 \), \( f_5(1.618035) < 0 \) for \( n \geq 3 \), \( f_5(\sqrt{n}) < 0 \) for \( n \geq 4 \), and \( f_5(\sqrt{n + 1}) > 0 \) for \( n \geq 10 \), we have

\[
E(Q^5_{2n}) < 2(n - 4) + 2(\sqrt{n + 1} + 1.618035 + 0.61806 + 0.01) \quad (n \geq 138589) . \quad (23)
\]

It follows from \( 2(n - 4) + 2(\sqrt{n + 1} + 1.618035 + 0.61806 + 0.01) < 2(n - 3) + 2(\sqrt{1.99} + \sqrt{n + 0.5}) \) that the RHS of (23) is less than the LHS of (22) as \( n \geq 138589 \). Therefore, \( Q^5_{2n} \to Q^4_{2n} \) for \( n \geq 138589 \). The calculation yields \( Q^5_{2n} \to Q^4_{2n} \) for \( 138588 \geq n \geq 40 \) while \( Q^4_{2n} \to Q^5_{2n} \) for \( 39 \geq n \geq 3 \). Therefore Lemma 7(ii) holds.

■

**Lemma 8.** \( Q^4_{2n} \to J^3_{2n} \) for \( n \geq 3 \).

**Proof.** It is noted that \( m(\hat{Q}^4_{2n}, 2) = m(X_n \cup P_2, 2) = n - 1 \). Since one 2-matching of \( \hat{Q}^4_{2n} \) are adjacent to two edges of \( M(Q^4_{2n}) \) and the other 2-matchings of \( \hat{Q}^4_{2n} \) to three edges of \( M(Q^4_{2n}) \), and \( m(\hat{Q}^4_{2n}, i) = 0 \) for \( 3 \leq i \leq n \), we have

\[
m(Q^4_{2n}, k) = p + \binom{n - 2}{k - 2} + (n - 2) \binom{n - 3}{k - 2} . \quad (24)
\]

From Lemma 3 and the fact that \( Q^4_{2n} - C_4 \) is composed of \( n - 2 \) independent edges,
From (25) and (26), we have

\begin{align*}
b_{2k}(Q^4_{2n}) &= m(Q^4_{2n}, k) - 2m(Q^4_{2n} - C_4, k - 2) \\
&= m(Q^4_{2n}, k) - 2 \left( \begin{array}{c} n - 2 \\ k - 2 \end{array} \right) \\
&= p - \left( \begin{array}{c} n - 2 \\ k - 2 \end{array} \right) + (n - 2) \left( \begin{array}{c} n - 3 \\ k - 2 \end{array} \right).
\end{align*}

(25)

Obviously, \(m(\widehat{J}^3_{2n}, 2) = m(Y_{n+1}, 2) = n - 2\). Since each 2-matching of \(\widehat{J}^3_{2n}\) are adjacent to three edges of \(M(J^3_{2n})\) and \(m(\widehat{J}^3_{2n}, i) = 0\) for \(3 \leq i \leq n\), from Lemma 3, we have

\[ b_{2k}(J^3_{2n}) = m(J^3_{2n}, k) = p + (n - 2) \left( \begin{array}{c} n - 3 \\ k - 2 \end{array} \right). \]

(26)

From (25) and (26), we have \(b_{2k}(Q^4_{2n}) \leq b_{2k}(J^3_{2n})\), where the equality does not hold for all \(k\). For example, \(b_4(Q^4_{2n}) < b_4(J^3_{2n})\). By Lemma 3, we have \(b_{2k}(Q^4_{2n}) = 0 \leq b_{2k+1}(J^3_{2n})\), where the equality does not hold for all \(k\). For example, \(b_3(Q^4_{2n}) = 0 < b_3(J^3_{2n}) = 2\). Thus, Lemma 8 holds.

**Lemma 9.** \(J^3_{2n} \rightarrow R^4_{2n}\) for \(n \geq 45\) and \(R^4_{2n} \rightarrow J^3_{2n}\) for \(44 \geq n \geq 4\).

**Proof.** Straightforward derivation by Lemma 1 yields

\begin{align*}
\phi(J^3_{2n}, x) &= (x^2 - 1)^{n-3} \left[ -1 + 2x + (1 + 2n)x^2 - 2x^3 - (3 + n)x^4 + x^6 \right] \\
&\triangleq (x^2 - 1)^{n-3} f_6(x) \quad (27) \\
\phi(R^4_{2n}, x) &= (x^2 - 1)^{n-4} \left[ 1 - (4 + n)x^2 + (-2 + 4n)x^4 - (4 + n)x^6 + x^8 \right] \\
&\triangleq (x^2 - 1)^{n-4} f_7(x) . \quad (28)
\end{align*}

Since \(f_6(-\sqrt{n + 1}) > 0\) for \(n \geq 3\), \(f_6(-\sqrt{n}) < 0\) for \(n \geq 3\), \(f_6(-1.4144) < 0\) for \(n \geq 3\), \(f_6(-1.4142) > 0\) for \(n \geq 2239\), \(f_6(-0.01) > 0\) for \(n \geq 5100\), \(f_6(-1/n) < 0\) for \(n \geq 3\), \(f_6(1/n) < 0\) for \(n \geq 5\), \(f_6(0.01) > 0\) for \(n \geq 4900\), \(f_6(1.4142) > 0\) for \(n \geq 75971\), \(f_6(1.4144) < 0\) for \(n \geq 3\), \(f_6(\sqrt{n}) < 0\) for \(n \geq 3\), and \(f_6(\sqrt{n + 2}) > 0\) for \(n \geq 7\), we have

\[ E(J^3_{2n}) < 2(n - 3) + \sqrt{n + 1} + 2(1.4144 + 0.01) + \sqrt{n + 2}, \quad (n \geq 75971). \]

(29)
Since $f_\tau(\sqrt{1/n^2}) > 0$ for $n \geq 3$, $f_\tau(\sqrt{0.01}) < 0$ for $n \geq 100$, $f_\tau(\sqrt{0.26791}) < 0$ for $n \geq 3$, $f_\tau(\sqrt{0.268}) > 0$ for $n \geq 6095$, $f_\tau(\sqrt{3.728761}) > 0$ for $n \geq 1315$, $f_\tau(\sqrt{3.732624}) < 0$ for $n \geq 3$, $f_\tau(\sqrt{n}) < 0$ for $n \geq 3$, and $f_\tau(\sqrt{n+1}) > 0$ for $n \geq 7$, we have

$$2(n - 4) + 2(1/n + \sqrt{0.26791} + \sqrt{3.728761} + \sqrt{n}) < E(R^4_{2n}) \quad (n \geq 6095). \quad (30)$$

It follows from $2(n - 3) + \sqrt{n + 1} + 2(1.4144 + 0.01) + \sqrt{n + 2} < 2(n - 4) + 2(1/n + \sqrt{0.26791} + \sqrt{3.728761} + \sqrt{n})$ that the RHS of (29) is less than the LHS of (30) as $n \geq 75971$. Therefore, $J^3_{2n} \rightarrow R^4_{2n}$ for $n \geq 75971$. The calculation yields $J^3_{2n} \rightarrow R^4_{2n}$ for $75970 \geq n \geq 45$ while $R^4_{2n} \rightarrow J^3_{2n}$ for $44 \geq n \geq 4$. ■

Let $\text{dia}(G - e)$ denote the diameter of $G - e$.

**Lemma 10.** Let $G \in K^l_{2n}$ with $n \geq 5$. If $G \neq R^3_{2n}, S^3_{2n}, Y^3_{2n}, J^3_{2n}, S^4_{2n}, Q^4_{2n}, Q^5_{2n}$, then $m(\hat{G}, 2) \geq 2n - 7$.

**Proof.** Let $G \in K^l_{2n}$ with $n \geq 5$. We consider three cases according to the types of the capped graph of $\hat{G}$.

(i) $\hat{G}$ is a connected unicyclic graph.

As $l \geq 4$ and $n \geq 5$, we can choose an edge $e$ on $C_1$ of $\hat{G}$ such that $\text{dia}(\hat{G} - e) \geq 4$. Therefore, $\hat{G} - e \neq X_n, Y_n, Z_n$ since $\text{dia}(X_n) = 2$ and $\text{dia}(Y_n) = \text{dia}(Z_n) = 3$. By Lemma 4, we have $m(\hat{G} - e, 2) \geq m(W_n, 2) = 2n - 7$. Furthermore, by Lemma 2, we have $m(\hat{G}, 2) \geq m(\hat{G} - e, 2) = 2n - 7$.

Let $l = 3$ and $n \geq 5$. If only one vertex $u_3$ on $C_3$ is attached by a tree and $G \neq R^3_{2n}$, then the tree attached at $u_3$ on $C_3$ of $\hat{G}$ is not a star. Therefore, $\text{dia}(\hat{G} - u_2u_3) \geq 4$. If at least two vertices $u_2$ and $u_3$ on $C_3$ are attached by trees, then we have $\text{dia}(\hat{G} - u_2u_3) \geq 4$. Similar to that for $l \geq 4$, we have $m(\hat{G}, 2) \geq 2n - 7$.

(ii) $\hat{G}$ is a tree.

It can readily be verified that $G = S^3_{2n}$ as $\hat{G} = X_{n+1}$ and $G = Y^3_{2n}, J^3_{2n}, S^4_{2n}$ as $\hat{G} = Y_{n+1}$. Therefore, if $G \neq S^3_{2n}, Y^3_{2n}, J^3_{2n}, S^4_{2n}$, then $\hat{G} \neq X_{n+1}, Y_{n+1}$. By Lemma 4, we have $m(\hat{G}, 2) \geq m(Z_{n+1}, 2) = 2n - 6$.

(iii) $\hat{G}$ is an unconnected graph whose components are trees and cycle or trees only.
If $\hat{G}$ is composed of trees and cycle, we might concatenate them together into a connected unicyclic graph, denoted by $\hat{G}_1$, in such a way that $\hat{G}_1 \neq \hat{R}_{2n}^2$. It is obvious that $m(\hat{G}, 2) > m(\hat{G}_1, 2)$. From (i), we can easily get that $m(\hat{G}, 2) > 2n - 7$.

If $\hat{G}$ is composed of trees only and $G \neq Q_{2n}^4, Q_{2n}^5$ (namely, $\hat{G} \neq X_n \cup P_2$), we might concatenate them together into a tree, denoted by $\hat{G}_2$, in such a way that $\hat{G}_2 \neq X_{n+1}, Y_{n+1}$. It is obvious that $m(\hat{G}, 2) > m(\hat{G}_2, 2)$. From (ii), we easily get that $m(\hat{G}, 2) > 2n - 6$.

From (i), (ii) and (iii), we obtain Lemma 10. ■

**Lemma 11.** Let $G \in \mathcal{K}_{2n}^1$ with $n \geq 5$ and $l = 2r + 1$ or $l = 4j + 2$, where $r$ and $j$ are integers with $r \geq 1$ and $j \geq 1$. If $G \neq R_{2n}^3, S_{2n}^3, Y_{2n}^3, J_{2n}^3, S_{2n}^4, Q_{2n}^4, Q_{2n}^5$, then $E(R_{2n}^4) < E(G)$.

**Proof.** It is noted that $m(\hat{R}_{2n}^4, 2) = 2n - 6$. Since each 2-matching of $\hat{R}_{2n}^4$ are adjacent to four edges of $M(R_{2n}^4)$ and $m(\hat{R}_{2n}^4, i) = 0$ for $3 \leq i \leq n$, we have

$$m(R_{2n}^4, k) = p + (2n - 6) \left( \frac{n - 4}{k - 2} \right).$$

From Lemma 3 and the fact that $R_{2n}^4 - C_4$ is composed of $n - 4$ independent edges and four isolated vertices, we obtain

$$b_{2k}(R_{2n}^4) = m(R_{2n}^4, k) - 2m(R_{2n}^4 - C_4, k - 2)$$

$$= m(R_{2n}^4, k) - 2 \left( \frac{n - 4}{k - 2} \right) = p + (2n - 8) \left( \frac{n - 4}{k - 2} \right).$$

As $l = 2r + 1$ or $l = 4j + 2$, from Lemma 3, we have

$$b_{2k}(G) \geq m(G, k) = p + m(\hat{G}, 2) \left( \frac{n - j}{k - 2} \right) + \sum_{i=3}^{n} m(\hat{G}, i) \left( \frac{n - j}{k - i} \right)$$

$$\geq p + m(\hat{G}, 2) \left( \frac{n - 4}{k - 2} \right).$$

As $G \neq R_{2n}^3, S_{2n}^3, Y_{2n}^3, J_{2n}^3, S_{2n}^4, Q_{2n}^4, Q_{2n}^5$ and $n \geq 5$, by Lemma 10, (32) and (33), we have $b_{2k}(R_{2n}^4) \leq b_{2k}(G)$, where the equality does not hold for all $k$. For example, $b_4(R_{2n}^4) < b_4(G)$. From Lemma 3, we have $b_{2k+1}(R_{2n}^4) = 0 \leq b_{2k+1}(G)$. Thus, Lemma 11 holds. ■
On the basis of Lemmas 5–11, we further extend Wang’s [11] and Li’s [12] results in Theorems 1–3, which give the preceding unicyclic graphs with perfect matchings in the increasing ordering by their energies within $k_{2n}$ for $n \geq 5$. Next, we assume that $G$ appearing in the last terms of all the inequalities does not contain the preceding terms.

**Theorem 1.** Let $G \in k_{2n}$ and $l = 2r + 1$ or $l = 4j + 2$. If $G \neq q_{2n}$, we have

$$S_{2n}^3 \rightarrow S_{2n}^4 \rightarrow R_{2n}^3 \rightarrow Y_{2n}^3 \rightarrow Q_{2n}^4 \rightarrow R_{2n}^4 \rightarrow G, \quad (n \geq 45).$$

**Proof.** Let $n \geq 45$. By Lemmas 5, 6, 7(i), 8, 9, and 11, we have Theorem 1. ■

It should be noted that the calculation and graphical representation allow us to make a conjecture that both $w_{2n}^4 \rightarrow S_{2n}^3$ and $y_{2n}^3 \rightarrow q_{2n}^5$ hold for $n \geq 3$, which, however, can not be proved by the theorem of zero points. By Lemma 7(ii), we have $q_{2n}^5 \rightarrow q_{2n}^4$ for $n \geq 40$. Therefore, we have Conjecture 1 as follows.

**Conjecture 1.** Let $G \in k_{2n}$ and $l = 2r + 1$ or $l = 4j + 2$. As $n \geq 45$, we have

$$w_{2n}^4 \rightarrow s_{2n}^3 \rightarrow s_{2n}^4 \rightarrow r_{2n}^3 \rightarrow y_{2n}^3 \rightarrow q_{2n}^5 \rightarrow q_{2n}^4 \rightarrow j_{2n}^3 \rightarrow r_{2n}^4 \rightarrow G.$$

The calculation yields

$$y_{2n}^3 \rightarrow q_{2n}^5 \rightarrow r_{2n}^4 \quad (44 \geq n \geq 10).$$

For the sake of conciseness, the symbol $(\bar{U})$ denotes (35) hereinafter.

**Theorem 2.** Let $G \in k_{2n}$ and $l = 2r + 1$ or $l = 4j + 2$. If $G \neq j_{2n}^3$, we have

$$w_{2n}^4 \rightarrow s_{2n}^3 \rightarrow s_{2n}^4 \rightarrow r_{2n}^3 \rightarrow y_{2n}^3 \rightarrow q_{2n}^5 \rightarrow q_{2n}^4 \rightarrow r_{2n}^4 \rightarrow G \quad (44 \geq n \geq 40) \quad (36)$$

$$w_{2n}^4 \rightarrow s_{2n}^3 \rightarrow s_{2n}^4 \rightarrow r_{2n}^3 \rightarrow y_{2n}^3 \rightarrow q_{2n}^4 \rightarrow q_{2n}^5 \rightarrow r_{2n}^4 \rightarrow G \quad (39 \geq n \geq 37) \quad (37)$$

$$w_{2n}^4 \rightarrow s_{2n}^3 \rightarrow s_{2n}^4 \rightarrow r_{2n}^3 \rightarrow q_{2n}^5 \rightarrow (\bar{U}) \rightarrow G \quad (36 \geq n \geq 33) \quad (38)$$

$$w_{2n}^4 \rightarrow s_{2n}^3 \rightarrow s_{2n}^4 \rightarrow q_{2n}^5 \rightarrow r_{2n}^3 \rightarrow (\bar{U}) \rightarrow G \quad (32 \geq n \geq 30) \quad (39)$$

$$w_{2n}^4 \rightarrow s_{2n}^3 \rightarrow q_{2n}^4 \rightarrow s_{2n}^4 \rightarrow r_{2n}^3 \rightarrow (\bar{U}) \rightarrow G \quad (29 \geq n \geq 14) \quad (40)$$

$$w_{2n}^4 \rightarrow q_{2n}^4 \rightarrow s_{2n}^3 \rightarrow s_{2n}^4 \rightarrow r_{2n}^3 \rightarrow (\bar{U}) \rightarrow G \quad (13 \geq n \geq 10). \quad (41)$$

**Proof.** By Lemma 5, we have $s_{2n}^3 \rightarrow s_{2n}^4$ in (36)–(39) and (41). By Lemma 6, we have $s_{2n}^4 \rightarrow r_{2n}^3 \rightarrow y_{2n}^3$ in (36), (37), (40), and (41), $s_{2n}^4 \rightarrow r_{2n}^3$ in (38) and $r_{2n}^3 \rightarrow y_{2n}^3$ in (39). By Lemma 11, we have $r_{2n}^4 \rightarrow G$ in (36)–(41).
The calculation yields $W_{2n}^4 ightarrow S_{2n}^3$ in (36)–(40), $Y_{2n}^3 ightarrow Q_{2n}^5 ightarrow Q_{2n}^4 ightarrow R_{2n}^3$ in (36), $Y_{2n}^3 ightarrow Q_{2n}^4 ightarrow Q_{2n}^5 ightarrow R_{2n}^3$ in (37), $R_{2n}^3 ightarrow Q_{2n}^4 ightarrow Y_{2n}^3$ in (38), $S_{2n}^3 ightarrow Q_{2n}^4 ightarrow R_{2n}^3$ in (39), $S_{2n}^3 ightarrow Q_{2n}^4 ightarrow S_{2n}^3$ in (40), and $W_{2n}^4 ightarrow Q_{2n}^4 ightarrow S_{2n}^3$ in (41).

**Theorem 3.** Let $G \in K_{2n}^l$ and $l = 2r + 1$ or $l = 4j + 2.$

(i) If $G \neq J_{2n}^3, Q_{2n}^5$, we have

$$W_{2n}^4 ightarrow Q_{2n}^4 ightarrow S_{2n}^3 ightarrow S_{2n}^4 ightarrow R_{2n}^3 ightarrow Y_{2n}^3 ightarrow R_{2n}^4 ightarrow G \quad (n = 9, 8).$$

(ii) If $G \neq Y_{2n}^3, J_{2n}^3, Q_{2n}^5$, we have

$$W_{2n}^4 ightarrow Q_{2n}^4 ightarrow S_{2n}^3 ightarrow S_{2n}^4 ightarrow R_{2n}^3 ightarrow R_{2n}^4 ightarrow G \quad (n = 7).$$

$$W_{2n}^4 ightarrow Q_{2n}^4 ightarrow S_{2n}^3 ightarrow S_{2n}^4 ightarrow R_{2n}^3 ightarrow R_{2n}^4 ightarrow G \quad (n = 6).$$

(iii) If $G \neq R_{2n}^3, Y_{2n}^3, J_{2n}^3, Q_{2n}^5$, we have

$$W_{2n}^4 ightarrow Q_{2n}^4 ightarrow S_{2n}^4 ightarrow S_{2n}^3 ightarrow R_{2n}^4 ightarrow G \quad (n = 5).$$

**Proof.** By Lemma 11, we have $R_{2n}^4 \rightarrow G$ in (42)–(45).

(i). By Lemmas 5 and 6, we have $S_{2n}^3 \rightarrow S_{2n}^4 \rightarrow R_{2n}^3 \rightarrow Y_{2n}^3$ in (42). As $n = 9, 8$, the calculation yields $W_{2n}^4 ightarrow Q_{2n}^4 ightarrow S_{2n}^3$ and $Y_{2n}^3 ightarrow R_{2n}^4$ in (42).

(ii). By Lemmas 5 and 6, we have $S_{2n}^3 \rightarrow S_{2n}^4 \rightarrow R_{2n}^3$ in (43). As $n = 7$, the calculation yields $W_{2n}^4 ightarrow Q_{2n}^4 ightarrow S_{2n}^3$ and $R_{2n}^3 \rightarrow R_{2n}^4$ in (43). As $n = 6$, the calculation yields $W_{2n}^4 ightarrow Q_{2n}^4 ightarrow S_{2n}^3 \rightarrow R_{2n}^3 \rightarrow R_{2n}^4$ in (44).

(iii). As $n = 5$, the calculation yields $W_{2n}^4 ightarrow Q_{2n}^4 \rightarrow S_{2n}^4 \rightarrow S_{2n}^3 \rightarrow R_{2n}^4$ in (45).

## 4 Conclusions

Using the method of coefficient comparison and the theorem of zero points, we studied the ordering of the unicyclic graphs with perfect matchings in terms of their minimal energies. In Theorems 1 and 2, we deduced the first 7 and 8 unicyclic graphs with perfect matchings for $n \geq 45$ and $44 \geq n \geq 10$, respectively. In Theorem 3, we listed the first 7, 6, and 5 unicyclic graphs with perfect matchings for $9 \geq n \geq 8$, $7 \geq n \geq 6$, and $n = 5$, respectively.
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References


