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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 π-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 $\mathbb{A}(G)$ its adjacent matrix. The characteristic polynomial of G is [24]

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

where $\mathbb{I}$ 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 π-electrons in conjugated hydrocarbons, within the framework of HMO approximation [1, 24], can be reduced to

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

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

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

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

$$b_i(G_1) \geq b_i(G_2) \ \Rightarrow \ E(G_1) \geq E(G_2) \tag{4}$$

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 " $\rightharpoonup$ ", " $\rightleftharpoons$ " and " $\rightrightarrows$ " as follows.

$$\begin{aligned} &E(G_1) < E(G_2) \iff G_1 \rightharpoonup G_2 \ , \quad E(G_1) = E(G_2) \iff G_1 \rightleftharpoons G_2 \\ &E(G_1) \leq E(G_2) \iff G_1 \rightrightarrows G_2 \ . \end{aligned} \tag{5}$$

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 $\widehat{G} = G - M(G) - S_0$, 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 $\widehat{G}$ the capped graph of G and G the original graph of $\widehat{G}$. Each k-matching Ω of G can be partitioned into two parts: $\Omega = \Phi \bigcup \Psi$, where Φ is a matching in $\widehat{G}$ and $\Psi \subset M(G)$.

Thus, we have [3]

$$m(G,k) = \sum_{i=0}^{k} m(\widehat{G},i) \binom{n-j}{k-i} = p + \sum_{i=2}^{k} m(\widehat{G},i) \binom{n-j}{k-i} \tag{6}$$

where

$$p = \binom{n}{k} + n \binom{n-2}{k-1}$$

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

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*

$$\phi(G) = \phi(G-e) - \phi(G-u-v) \ . \tag{7}$$

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

$$m(G,k) = m(G-e,k) + m(G-u-v,k-1) \ . \tag{8}$$

Lemma 3. [9, 11] *Let $G \in \mathcal{K}_{2n}^{l}$ 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 $0 \leq k \leq [n/2]$.*

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

Let R_{2n}^3 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_{2n}^3 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.

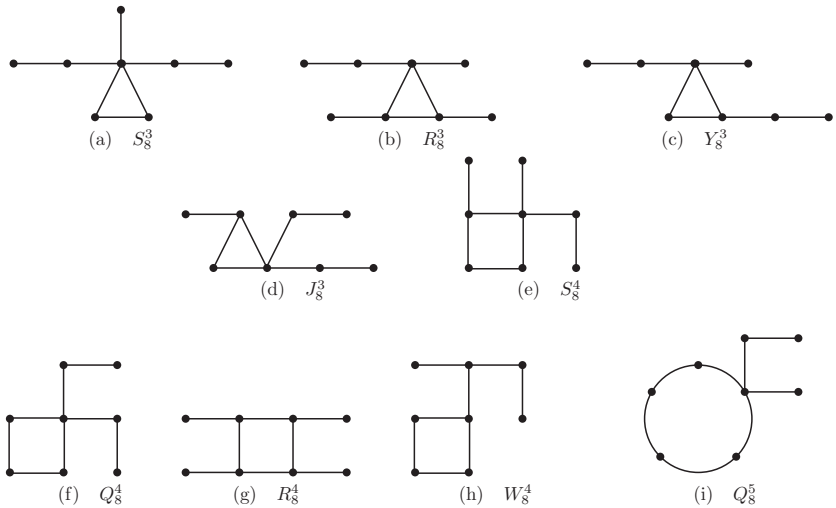

Figure 1: Some graphs with $n = 8$

Let J_{2n}^3 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_{2n}^4 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_{2n}^4 be the graph obtained from C_4 by attaching $n-2$ paths of length 2 to u_1.

Let R_{2n}^4 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_{2n}^4 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_{2n}^5 be the graph obtained from C_5 by attaching one pendant and $n-3$ paths of length 2 to u_1.

For example, S_8^3, R_8^3, Y_8^3, J_8^3, S_8^4, Q_8^4, R_8^4, W_8^4, and Q_8^5 are shown in Fig. 1.

Lemma 5. *$S_{2n}^3 \rightharpoonup S_{2n}^4$ for $n \geq 7$ and $S_{2n}^4 \rightharpoonup S_{2n}^3$ for $6 \geq n \geq 3$.*

Proof. Straightforward derivation by Lemma 1 yields

$$\begin{aligned}\phi(S_{2n}^3, x) &= (x^2-1)^{n-2}\left[1-2x-(2+n)x^2+x^4\right] \\ &\triangleq (x^2-1)^{n-2} f_1(x) \qquad (9)\\ \phi(S_{2n}^4, x) &= (x^2-1)^{n-4}\left[1-(3+n)x^2+(2+3n)x^4-(4+n)x^6+x^8\right] \\ &\triangleq (x^2-1)^{n-4} f_2(x)\ . \qquad (10)\end{aligned}$$

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_{2n}^3 and S_{2n}^4 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 $1\le i\le 4$.

Obviously, we have

$$\begin{aligned}
&f_1(-\sqrt{n+2}) = 1+2\sqrt{n+2}>0 && (n\ge 3)\\
&f_1(-\sqrt{n+1}) = -n+2\sqrt{n+1}<0 && (n\ge 5)\\
&f_1(-0.01) = 1.0198-0.0001n<0 && (n\ge 10199)\\
&f_1(-1/n) = 1+1/n^4-2/n^2+1/n>0 && (n\ge 3)\\
&f_1(1/n) = 1+1/n^4-2/n^2-3/n>0 && (n\ge 4)\\
&f_1(0.01) = 0.9798-0.0001n<0 && (n\ge 9798)\\
&f_1(\sqrt{n+1}) = -n-2\sqrt{1+n}<0 && (n\ge 3)\\
&f_1(\sqrt{n+3}) = 4+n-2\sqrt{3+n}>0 && (n\ge 3)\ .
\end{aligned}$$

According to the theorem of zero points, we have

$$\begin{aligned}E(S_{2n}^3) &= 2(n-2)+\sum_{i=1}^{4}|x_i| \\ &< 2(n-2)+\sqrt{n+2}+0.01+0.01+\sqrt{n+3}, \qquad (n\ge 10199)\ . \qquad (11)\end{aligned}$$

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

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

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, $S_{2n}^3 \rightharpoonup S_{2n}^4$ for $n \geq 10199$. The calculation yields $S_{2n}^3 \rightharpoonup S_{2n}^4$ for $10198 \geq n \geq 7$ while $S_{2n}^4 \rightharpoonup S_{2n}^3$ for $6 \geq n \geq 3$. ■

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

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

$$b_{2k}(S_{2n}^4) = p - \binom{n-3}{k-2} + (n-3)\binom{n-4}{k-2}. \tag{13}$$

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

$$b_{2k}(R_{2n}^3) = m(R_{2n}^3, k) = p + (n-3)\binom{n-4}{k-2}. \tag{14}$$

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

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

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

$$b_{2k}(Y_{2n}^3) = m(Y_{2n}^3, k) = p + \binom{n-3}{k-2} + (n-3)\binom{n-4}{k-2}. \tag{16}$$

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

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

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)* $Y_{2n}^3 \rightharpoonup Q_{2n}^4$ *for* $n \geq 37$ *and* $Q_{2n}^4 \rightharpoonup Y_{2n}^3$ *for* $36 \geq n \geq 3$.

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

Proof. Straightforward derivation by Lemma 1 yields

$$\begin{aligned} \phi(Y_{2n}^3, x) &= (x^2-1)^{n-4}\left[1 - 2x - (5+n)x^2 + 4x^3 + (4+3n)x^4 - 2x^5 - (4+n)x^6 + x^8\right] \\ &\triangleq (x^2-1)^{n-4} f_3(x) \qquad (18) \\ \phi(Q_{2n}^4, x) &= x^2(x^2-1)^{n-3}\left[2n - (3+n)x^2 + x^4\right] \\ &\triangleq x^2(x^2-1)^{n-3} f_4(x) \qquad (19) \\ \phi(Q_{2n}^5, x) &= (x^2-1)^{n-4}\left[1 + 2x - (6+n)x^2 - 2x^3 + (5+3n)x^4 - (4+n)x^6 + x^8\right] \\ &\triangleq (x^2-1)^{n-4} f_5(x)\ . \qquad (20) \end{aligned}$$

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

$$\begin{aligned} E(Y_{2n}^3) &< 2(n-4) + \sqrt{n+1} + 2(1.61804 + 0.61806 + 0.01) \\ &+ \sqrt{n+2} \qquad (n \geq 67715)\ . \end{aligned} \tag{21}$$

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

$$2(n-3) + 2(\sqrt{1.99} + \sqrt{n+0.5}) < E(Q_{2n}^4) \qquad (n \geq 201)\ . \tag{22}$$

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, $Y_{2n}^3 \rightharpoonup Q_{2n}^4$ for $n \geq 67715$. The calculation yields $Y_{2n}^3 \rightharpoonup Q_{2n}^4$ for $67714 \geq n \geq 37$ while $Q_{2n}^4 \rightharpoonup Y_{2n}^3$ 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 $n \geq 3$, $f_5(-1.618035) < 0$ for $n \geq 3$, $f_5(-1.61803) > 0$ for $n \geq 3$, $f_5(-0.61806) > 0$ for $n \geq 55637$, $f_5(-0.61803) < 0$ for $n \geq 3$, $f_5(-0.01) < 0$ for $n \geq 9797$, $f_5(-1/n) > 0$ for $n \geq 5$, $f_5(1/n) > 0$ for $n \geq 3$, $f_5(0.01) < 0$ for $n \geq 10198$, $f_5(0.61802) < 0$ 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

$$E(Q_{2n}^5) < 2(n-4) + 2(\sqrt{n+1} + 1.618035 + 0.61806 + 0.01) \qquad (n \geq 138589)\ . \tag{23}$$

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, $Q_{2n}^5 \rightharpoonup Q_{2n}^4$ for $n \geq 138589$. The calculation yields $Q_{2n}^5 \rightharpoonup Q_{2n}^4$ for $138588 \geq n \geq 40$ while $Q_{2n}^4 \rightharpoonup Q_{2n}^5$ for $39 \geq n \geq 3$. Therefore Lemma 7(ii) holds. ■

Lemma 8. *$Q_{2n}^4 \rightharpoonup J_{2n}^3$ for $n \geq 3$.*

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

$$m(Q_{2n}^4, k) = p + \binom{n-2}{k-2} + (n-2)\binom{n-3}{k-2}. \tag{24}$$

From Lemma 3 and the fact that $Q_{2n}^4 - C_4$ is composed of $n-2$ independent edges,

we obtain

$$\begin{aligned} b_{2k}(Q_{2n}^4) &= m(Q_{2n}^4, k) - 2m(Q_{2n}^4 - C_4, k-2) \\ &= m(Q_{2n}^4, k) - 2\begin{pmatrix} n-2 \\ k-2 \end{pmatrix} \\ &= p - \begin{pmatrix} n-2 \\ k-2 \end{pmatrix} + (n-2)\begin{pmatrix} n-3 \\ k-2 \end{pmatrix}. \end{aligned} \tag{25}$$

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

$$b_{2k}(J_{2n}^3) = m(J_{2n}^3, k) = p + (n-2)\begin{pmatrix} n-3 \\ k-2 \end{pmatrix}. \tag{26}$$

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

Lemma 9. *$J_{2n}^3 \rightharpoonup R_{2n}^4$ for $n \ge 45$ and $R_{2n}^4 \rightharpoonup J_{2n}^3$ for $44 \ge n \ge 4$.*

Proof. Straightforward derivation by Lemma 1 yields

$$\begin{aligned} \phi(J_{2n}^3, x) &= (x^2-1)^{n-3}\left[-1 + 2x + (1+2n)x^2 - 2x^3 - (3+n)x^4 + x^6\right] \\ &\triangleq (x^2-1)^{n-3} f_6(x) \end{aligned} \tag{27}$$

$$\begin{aligned} \phi(R_{2n}^4, x) &= (x^2-1)^{n-4}\left[1 - (4+n)x^2 + (-2+4n)x^4 - (4+n)x^6 + x^8\right] \\ &\triangleq (x^2-1)^{n-4} f_7(x)\ . \end{aligned} \tag{28}$$

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

$$E(J_{2n}^3) < 2(n-3) + \sqrt{n+1} + 2(1.4144 + 0.01) + \sqrt{n+2}, \quad (n \ge 75971). \tag{29}$$

Since $f_7(\sqrt{1/n^2}) > 0$ for $n \geq 3$, $f_7(\sqrt{0.01}) < 0$ for $n \geq 100$, $f_7(\sqrt{0.26791}) < 0$ for $n \geq 3$, $f_7(\sqrt{0.268}) > 0$ for $n \geq 6095$, $f_7(\sqrt{3.728761}) > 0$ for $n \geq 1315$, $f_7(\sqrt{3.732624}) < 0$ for $n \geq 3$, $f_7(\sqrt{n}) < 0$ for $n \geq 3$, and $f_7(\sqrt{n+1}) > 0$ for $n \geq 7$, we have

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

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, $J^3_{2n} \rightharpoonup R^4_{2n}$ for $n \geq 75971$. The calculation yields $J^3_{2n} \rightharpoonup R^4_{2n}$ for $75970 \geq n \geq 45$ while $R^4_{2n} \rightharpoonup J^3_{2n}$ for $44 \geq n \geq 4$. ■

Let $dia(G-e)$ denote the diameter of $G-e$.

Lemma 10. *Let $G \in \mathcal{K}^l_{2n}$ 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 $m(\widehat{G}, 2) \geq 2n-7$.*

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

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

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

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 $\widehat{G}$ is not a star. Therefore, $dia(\widehat{G} - u_2u_3) \geq 4$. If at least two vertices u_2 and u_3 on C_3 are attached by trees, then we have $dia(\widehat{G} - u_2u_3) \geq 4$. Similar to that for $l \geq 4$, we have $m(\widehat{G}, 2) \geq 2n-7$.

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

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

(iii) $\widehat{G}$ is an unconnected graph whose components are trees and cycle or trees only.

If $\widehat{G}$ is composed of trees and cycle, we might concatenate them together into a connected unicyclic graph, denoted by $\widehat{G}_1$, in such a way that $\widehat{G}_1 \neq \widehat{R}^3_{2n}$. It is obvious that $m(\widehat{G},2) > m(\widehat{G}_1,2)$. From (i), we can easily get that $m(\widehat{G},2) > 2n-7$.

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

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

Lemma 11. *Let $G \in \mathcal{K}^l_{2n}$ 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 $G \neq R^3_{2n}, S^3_{2n}, Y^3_{2n}, J^3_{2n}, S^4_{2n}, Q^4_{2n}, Q^5_{2n}$, then $E(R^4_{2n}) < E(G)$.*

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

$$m(R^4_{2n},k) = p + (2n-6)\begin{pmatrix} n-4 \\ k-2 \end{pmatrix}. \tag{31}$$

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

$$\begin{aligned} b_{2k}(R^4_{2n}) &= m(R^4_{2n},k) - 2m(R^4_{2n} - C_4, k-2) \\ &= m(R^4_{2n},k) - 2\begin{pmatrix} n-4 \\ k-2 \end{pmatrix} = p + (2n-8)\begin{pmatrix} n-4 \\ k-2 \end{pmatrix}. \end{aligned} \tag{32}$$

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

$$\begin{aligned} b_{2k}(G) \geq m(G,k) &= p + m(\widehat{G},2)\begin{pmatrix} n-j \\ k-2 \end{pmatrix} + \sum_{i=3}^{n} m(\widehat{G},i)\begin{pmatrix} n-j \\ k-i \end{pmatrix} \\ &\geq p + m(\widehat{G},2)\begin{pmatrix} n-4 \\ k-2 \end{pmatrix}. \end{aligned} \tag{33}$$

As $G \neq R^3_{2n}, S^3_{2n}, Y^3_{2n}, J^3_{2n}, S^4_{2n}, Q^4_{2n}, Q^5_{2n}$ and $n \geq 5$, by Lemma 10, (32) and (33), we have $b_{2k}(R^4_{2n}) \leq b_{2k}(G)$, where the equality does not hold for all k. For example, $b_4(R^4_{2n}) < b_4(G)$. From Lemma 3, we have $b_{2k+1}(R^4_{2n}) = 0 \leq b_{2k+1}(G)$. 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 $\mathcal{K}_{2n}^{l}$ 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 $G \in \mathcal{K}_{2n}^{l}$ and $l = 2r+1$ or $l = 4j+2$. If $G \neq Q_{2n}^{5}$, we have*

$$S_{2n}^{3} \rightharpoonup S_{2n}^{4} \rightharpoonup R_{2n}^{3} \rightharpoonup Y_{2n}^{3} \rightharpoonup Q_{2n}^{4} \rightharpoonup J_{2n}^{3} \rightharpoonup R_{2n}^{4} \rightharpoonup G, \qquad (n \geq 45). \tag{34}$$

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 $W_{2n}^{4} \rightharpoonup S_{2n}^{3}$ and $Y_{2n}^{3} \rightharpoonup Q_{2n}^{5}$ hold for $n \geq 3$, which, however, can not be proved by the theorem of zero points. By Lemma 7(ii), we have $Q_{2n}^{5} \rightharpoonup Q_{2n}^{4}$ for $n \geq 40$. Therefore, we have Conjecture 1 as follows.

Conjecture 1. *Let $G \in \mathcal{K}_{2n}^{l}$ and $l = 2r+1$ or $l = 4j+2$. As $n \geq 45$, we have $W_{2n}^{4} \rightharpoonup S_{2n}^{3} \rightharpoonup S_{2n}^{4} \rightharpoonup R_{2n}^{3} \rightharpoonup Y_{2n}^{3} \rightharpoonup Q_{2n}^{5} \rightharpoonup Q_{2n}^{4} \rightharpoonup J_{2n}^{3} \rightharpoonup R_{2n}^{4} \rightharpoonup G$.*

The calculation yields

$$Y_{2n}^{3} \rightharpoonup Q_{2n}^{5} \rightharpoonup R_{2n}^{4} \qquad (44 \geq n \geq 10). \tag{35}$$

For the sake of conciseness, the symbol $(\mho)$ denotes (35) hereinafter.

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

$$W_{2n}^{4} \rightharpoonup S_{2n}^{3} \rightharpoonup S_{2n}^{4} \rightharpoonup R_{2n}^{3} \rightharpoonup Y_{2n}^{3} \rightharpoonup Q_{2n}^{5} \rightharpoonup Q_{2n}^{4} \rightharpoonup R_{2n}^{4} \rightharpoonup G \quad (44 \geq n \geq 40) \tag{36}$$

$$W_{2n}^{4} \rightharpoonup S_{2n}^{3} \rightharpoonup S_{2n}^{4} \rightharpoonup R_{2n}^{3} \rightharpoonup Y_{2n}^{3} \rightharpoonup Q_{2n}^{4} \rightharpoonup Q_{2n}^{5} \rightharpoonup R_{2n}^{4} \rightharpoonup G \quad (39 \geq n \geq 37) \tag{37}$$

$$W_{2n}^{4} \rightharpoonup S_{2n}^{3} \rightharpoonup S_{2n}^{4} \rightharpoonup R_{2n}^{3} \rightharpoonup Q_{2n}^{4} \rightharpoonup (\mho) \rightharpoonup G \quad (36 \geq n \geq 33) \tag{38}$$

$$W_{2n}^{4} \rightharpoonup S_{2n}^{3} \rightharpoonup S_{2n}^{4} \rightharpoonup Q_{2n}^{4} \rightharpoonup R_{2n}^{3} \rightharpoonup (\mho) \rightharpoonup G \quad (32 \geq n \geq 30) \tag{39}$$

$$W_{2n}^{4} \rightharpoonup S_{2n}^{3} \rightharpoonup Q_{2n}^{4} \rightharpoonup S_{2n}^{4} \rightharpoonup R_{2n}^{3} \rightharpoonup (\mho) \rightharpoonup G \quad (29 \geq n \geq 14) \tag{40}$$

$$W_{2n}^{4} \rightharpoonup Q_{2n}^{4} \rightharpoonup S_{2n}^{3} \rightharpoonup S_{2n}^{4} \rightharpoonup R_{2n}^{3} \rightharpoonup (\mho) \rightharpoonup G \quad (13 \geq n \geq 10)\ . \tag{41}$$

Proof. By Lemma 5, we have $S_{2n}^{3} \rightharpoonup S_{2n}^{4}$ in (36)–(39) and (41). By Lemma 6, we have $S_{2n}^{4} \rightharpoonup R_{2n}^{3} \rightharpoonup Y_{2n}^{3}$ in (36), (37), (40), and (41), $S_{2n}^{4} \rightharpoonup R_{2n}^{3}$ in (38) and $R_{2n}^{3} \rightharpoonup Y_{2n}^{3}$ in (39). By Lemma 11, we have $R_{2n}^{4} \rightharpoonup G$ in (36)– (41).

The calculation yields $W_{2n}^4 \rightharpoonup S_{2n}^3$ in (36)–(40), $Y_{2n}^3 \rightharpoonup Q_{2n}^5 \rightharpoonup Q_{2n}^4 \rightharpoonup R_{2n}^4$ in (36), $Y_{2n}^3 \rightharpoonup Q_{2n}^4 \rightharpoonup Q_{2n}^5 \rightharpoonup R_{2n}^4$ in (37), $R_{2n}^3 \rightharpoonup Q_{2n}^4 \rightharpoonup Y_{2n}^3$ in (38), $S_{2n}^4 \rightharpoonup Q_{2n}^4 \rightharpoonup R_{2n}^3$ in (39), $S_{2n}^3 \rightharpoonup Q_{2n}^4 \rightharpoonup S_{2n}^4$ in (40), and $W_{2n}^4 \rightharpoonup Q_{2n}^4 \rightharpoonup S_{2n}^3$ in (41). ■

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

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

$$W_{2n}^4 \rightharpoonup Q_{2n}^4 \rightharpoonup S_{2n}^3 \rightharpoonup S_{2n}^4 \rightharpoonup R_{2n}^3 \rightharpoonup Y_{2n}^3 \rightharpoonup R_{2n}^4 \rightharpoonup G \qquad (n = 9, 8)\ . \tag{42}$$

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

$$W_{2n}^4 \rightharpoonup Q_{2n}^4 \rightharpoonup S_{2n}^3 \rightharpoonup S_{2n}^4 \rightharpoonup R_{2n}^3 \rightharpoonup R_{2n}^4 \rightharpoonup G \qquad (n = 7) \tag{43}$$

$$W_{2n}^4 \rightharpoonup Q_{2n}^4 \rightharpoonup S_{2n}^4 \rightharpoonup S_{2n}^3 \rightharpoonup R_{2n}^3 \rightharpoonup R_{2n}^4 \rightharpoonup G \qquad (n = 6)\ . \tag{44}$$

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

$$W_{2n}^4 \rightharpoonup Q_{2n}^4 \rightharpoonup S_{2n}^4 \rightharpoonup S_{2n}^3 \rightharpoonup R_{2n}^4 \rightharpoonup G \qquad (n = 5)\ . \tag{45}$$

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

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

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

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