On minimal energy ordering of acyclic conjugated molecules

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The energy of a graph is defined as the sum of the absolute values of all the eigenvalues of the graph. Gutman (Acyclic conjugated molecules, trees and their energies, J. Math. Chem. 1 (1987) 123–143) proposes two conjectures about the minimum of the energy of conjugated trees (trees with a perfect matching), which are verified by Zhang and Li (On acyclic conjugated molecules with minimal energies, Discrete Appl. Math. 92 (1999) 71–84). This paper focuses on the trees of conjugated hydrocarbons and gives roughly the first $n/2$ trees in the class in the increasing order of their energies.

1. Introduction

Chemists have known that the experimental heats of formation of conjugated hydrocarbons are closely related to the total π-electron energy. And the calculation of the total energy of all π-electrons in a conjugated hydrocarbon can be reduced (within the framework of the HMO approximation) [4] to

$$E(T) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|,$$

where λ_i are the eigenvalues of the corresponding graph. For an acyclic (or tree) graph T this energy is also expressible in terms of the Coulson integral formula [4] as

$$E(T) = \frac{2}{\pi}\int_0^{+\infty} x^{-2}\ln\left[1+\sum_{k=1}^{n/2} m(T,k)x^{2k}\right]\mathrm{d}x,$$

where $m(T,k)$ is the number of k-matchings of T. The fact that $E(T)$ is a strictly monotonically increasing function of all matching numbers $m(T,k)$, $k = 0, 1, \ldots, \lfloor n/2\rfloor$, provides us with a way of comparing the energies of trees. Thus a quasi-ordering is introduced: if for two graphs G_1 and G_2, $m(G_1,k) \leqslant m(G_2,k)$ holds for all $k \geqslant 0$, we say G_1 is m-*smaller* than G_2, written as $G_1 \preceq G_2$ or $G_2 \succeq G_1$. G_1 and G_2 are m-*equivalent*, written as $G_1 \sim G_2$, if $G_1 \preceq G_2$ and $G_2 \preceq G_1$. If $G_1 \preceq G_2$ but they are not m-equivalent, then $G_1 \prec G_2$. If neither $G_1 \preceq G_2$ nor $G_2 \preceq G_1$, then

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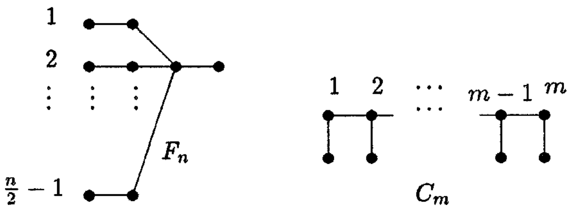


Figure 1. F_n and C_m.

G_1 and G_2 are said to be *m-incomparable*. By the monotonicity of $E(T)$, if $T_1 \preceq T_2$ for two trees T_1 and T_2, then $E(T_1) \leqslant E(T_2)$, and $E(T_1) < E(T_2)$ if $T_1 \prec T_2$. For the study of a quasiordering a number of results have been reached [2,5–9]. A typical one [5], which we frequently use, is that if we denote by $G \cup H$ the graph whose components are G and H, then

$$\begin{aligned} P_l &\succeq P_2 \cup P_{l-2} \succeq P_4 \cup P_{l-4} \succeq \cdots \succeq P_{2k} \cup P_{l-2k} \succeq P_{2k+1} \cup P_{l-2k-1} \\ &\succeq P_{2k-1} \cup P_{l-2k+1} \succeq \cdots \succeq P_3 \cup P_{l-3} \succeq P_1 \cup P_{l-1}, \end{aligned}$$

where P_i is the path with i vertices and $l = 4k + r,\ 0 \leqslant r \leqslant 3$.

For the case of minimal energy, Gutman has put forward the following two conjectures [3].

Conjecture 1. Among trees of n vertices which have a perfect matching, $E(T)$ is minimal for the graph F_n, where F_n is obtained by adding a pendant edge to each vertex of the star $K_{1,n/2-1}$.

Conjecture 2. Among trees with $n = 2m$ vertices which have a perfect matching and whose vertex degrees do not exceed 3, $E(T)$ is minimal for the comb C_m obtained by adding a pendant edge to each vertex of the path P_m (see figure 1).

He has also checked all the trees with a perfect matching less than sixteen vertices.

In [10], Zhang and the present author have verified the above two conjectures using the quasiordering relation $\prec$. And we went further to give the second smallest tree and show that the third smallest is between two trees, which $\prec$ fails to compare. That tells us that we have reached a blind alley through the quasiordering relation $\prec$ to order the trees in terms of their energies in the class of trees with a perfect matching. It is curious enough, however, that in this paper a fairly long series is determined in the ordering of trees with a perfect matching whose vertex degrees do not exceed 3. And the series is still open ended in the searching. The proofs are given in the following sections.

2. Preliminaries

Denote by Φ_n the class of trees with n vertices which have a perfect matching and by Ψ_n the subclass of Φ_n whose vertex degrees do not exceed 3. Let $\Delta(G)$ be the largest vertex degree of the graph G.

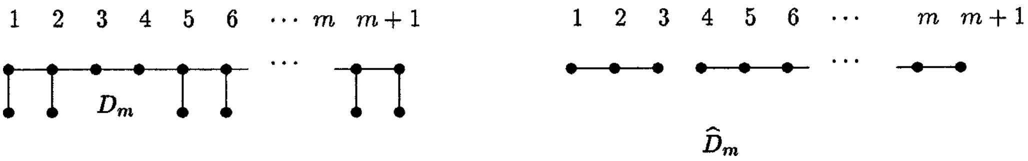


Figure 2. D_m and $\widehat{D}_m$.

Because the perfect matching of a tree T is unique, we denote it by $M(T)$. Let $m = |M(T)|$, $Q(T) = L(T) - M(T)$, where $L(T)$ is the edge set of T. Denote by $\widehat{T}$ the graph induced by $Q(T)$, that is, $\widehat{T} = T - M(T) - S$, where S is the set of singletons in $T - M(T)$. We call $\widehat{T}$ the *capped graph* of T and T an *original* or *uncapped graph* of $\widehat{T}$. For example, figure 2 shows the capped graph of D_m.

Each k-matching Ω of T is partitioned into two parts: $\Omega = R \cup S$, where $S \subseteq M(T)$ and R is a matching in $\widehat{T}$. On the other hand, any i-matching R of $\widehat{T}$ and $k - i$ edges S of $M(T)$ not incident with R form a k-matching Ω of T with partition $\Omega = R \cup S$. From now on, when we say a k-matching of T including a certain s-matching R of $\widehat{T}$, it is in such a sense. This is our fundamental principle of counting the k-matchings of T.

For convenience we extend the meaning of $m(G, k)$ by defining that $m(G, k) = 0$, if $k < 0$ and $m(G, 0) = 1$. So for all integers $k \in Z$, $m(G, k)$ is well-defined.

In Ψ_n, the capped graph $\widehat{T}$ of any tree T is unique and composed of disjoint paths with altogether $n/2 - 1$ edges:

$$\widehat{T} = P_{i_1} \cup P_{i_2} \cup \cdots \cup P_{i_r}, \quad i_\alpha > 1,\ \alpha = 1, 2, \ldots, r,$$

where $r = c(\widehat{T})$ is the number of connected components. And there is a unique set E of $M(T)$, called the *set of linking edges*, such that $\widehat{T} + E$ forms a tree of the same vertices as $\widehat{T}$ (equivalently, $\widehat{T}$ is incident with both end vertices of any edge e in E).

Conversely, for any graph U of disjoint paths of length greater than 0 with altogether $m - 1$ edges and a set E of disjoint edges such that $U + E$ forms a tree of the same vertices as U, there is a unique tree T in Ψ_n, formed by the principle of attaching a pendant edge to each vertex of $U + E$ except for the end vertices of the edges of E. Then $\widehat{T} = U$ and E is the set of linking edges. This process is shown in figure 3. The unique tree T is denoted by $T = T(U, E)$ and called the *uncapped graph* of U with respect to E. Hence suitable $\widehat{T}$ and E together are in one-to-one correspondence with T.

Let R be a matching of $\widehat{T}$, and $t(R)$ the number of edges e in $M(T)$ such that both end vertices of each such e are incident with R in T. Denote by $\beta_t(\widehat{T}, s)$ the number of s-matchings of $\widehat{T}$ incident with both end vertices of exactly t edges of $M(T)$, $t \geqslant 0$, where we define $\beta_0(\widehat{T}, 0) = 1$, $\beta_t(\widehat{T}, 0) = 0$ if $t > 0$, $\beta_t(\widehat{T}, s) = 0$ if $s < 0$, $t \geqslant 0$.

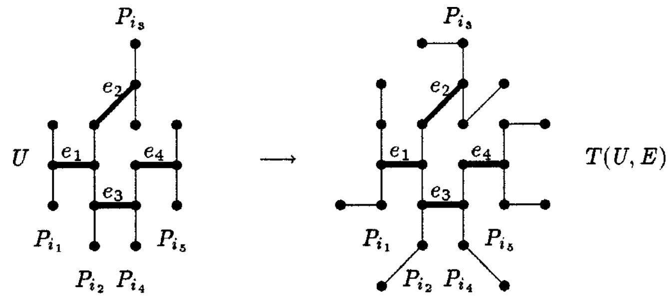


Figure 3. An example of the determination of $T(U,E)$ by U, where $r=5$ and $E=\{e_1,e_2,e_3,e_4\}$.

Lemma 1.

$$m(T,k) = \sum_{\substack{0\leqslant s\leqslant k\\ R \text{ is an } s\text{-matching of } \widehat{T}}} \binom{m-2s+t(R)}{k-s}, \quad k\in Z, \tag{1}$$

$$= \sum_{0\leqslant s\leqslant k}\sum_{0\leqslant t\leqslant m} \beta_t\bigl(\widehat{T},s\bigr)\binom{m-2s+t}{k-s}, \quad k\in Z, \tag{2}$$

where a 0-matching is $\emptyset$ and $t(\emptyset)=0$.

Proof. A k-matching Ω of T can be partitioned into two parts: $\Omega = R\cup S$, with $R\subseteq \widehat{T}$ and $S\subseteq M(T)$. The number of such k-matchings Ω with a fixed R is

$$\binom{m-2s+t(R)}{k-s},$$

which gives the first part of the equations. The second part is a straightforward derivation of the first. □

Because

$$\sum_{t=0}^{m}\beta_t\bigl(\widehat{T},s\bigr) = m\bigl(\widehat{T},s\bigr), \quad s\in Z, \tag{3}$$

we have

Lemma 2. If $m(\widehat{T}_1,s)\geqslant m(\widehat{T}_2,s)$ and $\beta_t(\widehat{T}_1,s)\geqslant\beta_t(\widehat{T}_2,s)$ for $t>0$, then $T_1\succeq T_2$. Also, $T_1\succ T_2$ if one of the previous inequalities is sharp.

Proof. By lemma 1,

$$m(T_1,k)-m(T_2,k) = \sum_{0\leqslant s\leqslant k}\sum_{0\leqslant t\leqslant m}\bigl[\beta_t\bigl(\widehat{T}_1,s\bigr)-\beta_t\bigl(\widehat{T}_2,s\bigr)\bigr]\binom{m-2s+t}{k-s}$$
$$\geqslant \sum_{0\leqslant s\leqslant k}\sum_{0\leqslant t\leqslant m}\bigl[\beta_t\bigl(\widehat{T}_1,s\bigr)-\beta_t\bigl(\widehat{T}_2,s\bigr)\bigr]\binom{m-2s}{k-s}$$

$$= \sum_{0\leqslant s\leqslant k} \left[m(\widehat{T}_1, s) - m(\widehat{T}_2, s)\right] \binom{m-2s}{k-s}$$
$$\geqslant 0. \qquad \square$$

Now we drop some edges E' from E and concatenate some paths in U into one by coalescing suitable pairs of their end vertices (by "suitable" we mean avoiding the end vertices of edges in $E - E'$) such that the graph U^* of the resulting disjoint paths together with the new linking edges $E - E'$ remains a tree. The process is shown in figure 4, where $r = 5$, $E = \{e_1, e_2, e_3, e_4\}$, $E' = \{e_1, e_3\}$ and $E - E' = \{e_2, e_4\}$. In the figure, we have concatenated P_{i_2}, P_{i_5} and P_{i_1}, respectively, at their end vertices but avoiding the end vertices of e_2 and e_4. We call the process a *concatenation* of U and the resulting graph of disjoint paths U^* is called a *concatenated graph* from U with respect to $E - E'$. (In the figure, $U^* = P_3 \cup P_3 \cup P_8$.) We have

Lemma 3. $T(U, E) \succ T(U^*, E - E')$.

Proof. We denote $T(U, E)$ by T and $T(U^*, E - E')$ by T^*. We note that the capped graphs of T and T^* are U and U^*, respectively, and U and U^* have the same edges. If two edges are incident in U, so are they in U^*. As a result, any s-matching R of U^* is also an s-matching of U. Therefore $U \succ U^*$, since there is a 2-matching of U which is a not a matching of U^* at all after the concatenation. In addition, if both end vertices of an edge e of the unique perfect matching $M(T) = M(T^*)$ is incident with two edges of a matching R of U^*, so is it with the same two edges of R of U on the grounds that the concatenation does not change the status of the end vertices of $E - E'$, to which e belongs. (The real difference between $M(T)$ and $M(T^*)$ is that none of the edges in E' is a pendant edge in T, while any of the edges in E' is in T^*.) Consequently, $t(R)$ in T^* is no larger than $t(R)$ in T. Finally, using the first part of the equations in lemma 1, we get $T^* \prec T$. $\square$

Next we show some orderings within the class of graphs whose capped graphs are composed of just two paths.

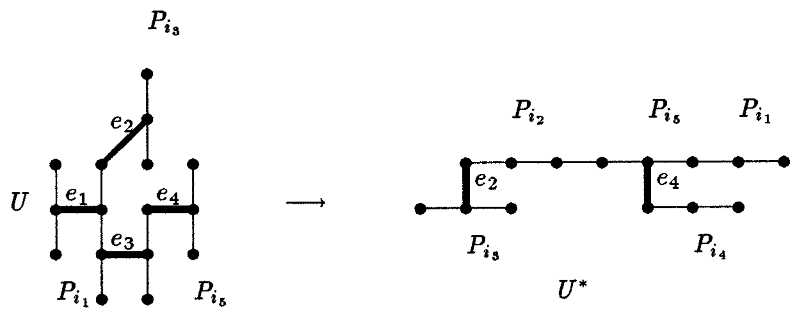


Figure 4. An example of the process of concatenation of the graph U, where $r = 5$, $E = \{e_1, e_2, e_3, e_4\}$, and $E' = \{e_1, e_3\}$.

3. Trees of 2-component capped graphs

Let $P_0 = \emptyset$, $J_a^c = P_a \cup P_b$, $P_a = u_1 \cdots u_a$, $P_b = v_1 \cdots v_b$, $a + b = c \geqslant 0$, $0 \leqslant a \leqslant \lfloor c/2 \rfloor = q$. Define $m(J_{-1}^c, k) = m(P_{-1} \cup P_{c+1}, k) = 0$, $k \in Z$. Denote $T_{i,j}^c(a) = T(J_a^c, u_i v_j)$ (we simply use the symbol $u_i v_j$ for $\{u_i v_j\}$ where there is no confusion), $2 \leqslant a \leqslant \lfloor c/2 \rfloor$, $1 \leqslant i \leqslant \lfloor (a+1)/2 \rfloor$, $1 \leqslant j \leqslant \lfloor (b+1)/2 \rfloor$, and $i \equiv p(q)$ instead of "i equals p modulo q".

Theorem 4.

(1) $J_1^c \prec J_3^c \prec \cdots \prec \cdots \prec \cdots \prec J_4^c \prec J_2^c \prec J_0^c$.

(2) $T_{1,1}^c(1) \prec T_{1,1}^c(3) \prec \cdots \prec \cdots \prec \cdots \prec T_{1,1}^c(4) \prec T_{1,1}^c(2)$, where $T_{1,1}^c(1) = T(J_1^c, u_1 v_1) = T(J_0^{c-1}, \emptyset)$ is also denoted by C_{c-1}.

Explanation: the series of (2) in this theorem is of the form $T_{1,1}^c(i)$ which is formed by omitting the ith and the $(i+1)$th teeth of the comb C_{m+1} with i ranging from 1 to $\lfloor (1/2)(m+1) \rfloor$. It is partitioned accordingly as whether i is odd or even. The odd part goes increasingly with i and the even part follows the odd part going in the inverse order of i. The series of (1) in this theorem is ordered in the same way, that is, accordingly as whether i, the subscript of J_i^c ranging from 0 to $\lfloor c/2 \rfloor$, is odd or even. The odd part goes increasingly with i and the even part follows the odd part going in the inverse order of i.

Before proving this theorem, we need two lemmas.

Lemma 5. Let $e = uv$ be an edge of a graph G, then

$$m(G, k) = m(G - e, k) + m(G - u - v, k - 1), \quad k \in Z. \tag{4}$$

The proof of this lemma can be found in many graph theory textbooks.

Lemma 6. Let G and H be two graphs. Denote by $G(u)H(v)$ the graph obtained by coalescing the vertex u of G and the vertex v of H. Suppose u and v are not singletons. Then

$$m(G \cup H, k) = m\big(G(u)H(v), k\big) + \sum_{\substack{uu_i \in G,\\ vv_j \in H}} m\big((G - u - u_i) \cup (H - v - v_j), k - 2\big), \quad k \in Z. \tag{5}$$

Proof. The k-matchings of $G \cup H$ are partitioned into two parts: those incident with both u and v, and those not, whose numbers are just the two terms on the right hand in the above equation. □

Proof of theorem 4. By the above two lemmas,

$$
\begin{aligned}
&m\bigl(J_i^c, s\bigr) - m\bigl(J_{i-2}^c, s\bigr)\\
&\quad = m(P_i \cup P_{c-i}, s) - m(P_{i-2} \cup P_{c-i+2}, s)\\
&\quad \overset{\text{lemma 6}}{=} m(P_{i-2} \cup P_{c-i-2}, s-2) - m(P_{i-4} \cup P_{c-i}, s-2) \overset{\text{lemma 6}}{=} \cdots \overset{\text{lemma 6}}{=}\\
&\quad \overset{\text{lemma 6}}{=} \begin{cases} m(P_2 \cup P_{c-2i+2}, s-i+2) - m(P_0 \cup P_{c-2i+4}, s-i+2), & i \equiv 0(2),\\ m(P_3 \cup P_{c-2i+3}, s-i+3) - m(P_1 \cup P_{c-2i+5}, s-i+3), & i \equiv 1(2), \end{cases}\\
&\quad \overset{\text{lemmas 5, 6}}{=} \begin{cases} -m(P_1 \cup P_{c-2i+1}, s-i+1) = -m(P_{c-2i+1}, s-i+1) \leqslant 0,\\ \quad i \equiv 0(2),\\ m(P_1 \cup P_{c-2i+1}, s-i+1) = m(P_{c-2i+1}, s-i+1) \geqslant 0,\\ \quad i \equiv 1(2), \end{cases}
\end{aligned}
\tag{6}
$$

$1 \leqslant i \leqslant q = \lfloor c/2 \rfloor$, $s \in Z$. When $s = i-1$, the last inequalities in (6) are sharp. And likewise,

$$
\begin{aligned}
&m\bigl(J_q^c, s\bigr) - m\bigl(J_{q-1}^c, s\bigr)\\
&\quad = m(P_q \cup P_{c-q}, s) - m(P_{q-1} \cup P_{c-q+1}, s) \overset{\text{lemma 6}}{=} \cdots \overset{\text{lemma 6}}{=}\\
&\quad \overset{\text{lemma 6}}{=} \begin{cases} m(P_2 \cup P_{c-2q+2}, s-q+2) - m(P_1 \cup P_{c-2q+3}, s-q+2)\\ m(P_1 \cup P_{c-2q+1}, s-q+1) - m(P_0 \cup P_{c-2q+2}, s-q+1) \end{cases}\\
&\quad \overset{\text{lemmas 5, 6}}{=} \begin{cases} m(P_{c-2q}, s-q) \geqslant 0, & q \equiv 0(2),\\ -m(P_{c-2q}, s-q) \leqslant 0, & q \equiv 1(2), \end{cases} \quad s \in Z.
\end{aligned}
\tag{7}
$$

When $s = q$, these inequalities are sharp. Thus (1) holds.

To show (2), it suffices to show, by lemma 2, that

$$
\beta_1\bigl(\widehat{T}_{1,1}^c(i), s\bigr) - \beta_1\bigl(\widehat{T}_{1,1}^c(i-2), s\bigr) \begin{cases} \leqslant 0, & i \equiv 0(2),\\ \geqslant 0, & i \equiv 1(2), \end{cases} \quad 3 \leqslant i \leqslant q,\ s \in Z,
$$

and

$$
\beta_1\bigl(\widehat{T}_{1,1}^c(q), s\bigr) - \beta_1\bigl(\widehat{T}_{1,1}^c(q-1), s\bigr) \begin{cases} \geqslant 0, & q \equiv 0(2),\\ \leqslant 0, & q \equiv 1(2), \end{cases} \quad s \in Z,
$$

$$
\beta_1(C_{c-1}, s) = 0. \quad \text{(This is evident.)}
$$

Now

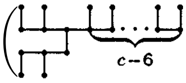
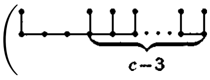
$$
\begin{aligned}
&\beta_1\bigl(\widehat{T}_{1,1}^c(i), s\bigr) - \beta_1\bigl(\widehat{T}_{1,1}^c(i-2), s\bigr)\\
&\quad = m(P_{i-2} \cup P_{c-i-2}, s-2) - m(P_{i-4} \cup P_{c-i}, s-2),\\
&\beta_1\bigl(\widehat{T}_{1,1}^c(q), s\bigr) - \beta_1\bigl(\widehat{T}_{1,1}^c(q-1), s\bigr)\\
&\quad = m(P_{q-2} \cup P_{c-q-2}, s-2) - m(P_{q-3} \cup P_{c-q-1}, s-2).
\end{aligned}
$$

Applying (6) and (7), we obtain the desired result. □

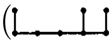
Theorem 7. $T_{1,1}^c(2) \prec T_{1,3}^c(3)$, $c \geqslant 8$.

Proof. We count the difference between the numbers of the k-matchings of the two graphs:

$m\big(T^c_{1,3}(3), k\big) - m\big(T^c_{1,1}(2), k\big)$

$= m\Big($  $, k\Big) - m\Big($  $, k\Big)$

$\overset{\text{lemma 5}}{=} \big[m\big($  $\big) \cup C_{c-6}, k\big) + m\big($  $\cup C_2 \cup C_{c-7}, k-1\big)\big]$

$- \big[m\big($  $\cup C_{c-6}, k\big) + m\big($  $\cup C_{c-7}, k-1\big)\big]$

$\overset{\text{lemma 5}}{=} \big[m(C_3 \cup C_2 \cup C_{c-6}, k) + m\big($  $\cup C_1 \cup C_{c-6}, k-1\big)\big]$

$$
\begin{aligned}
&+ \big[\underline{m(C_2 \cup C_2 \cup C_{c-7}, k-1)} + m(C_2 \cup C_1 \cup C_{c-7}, k-2)\big]\\
&- \big[m(P_6 \cup C_2 \cup C_{c-6}, k) + m(C_2 \cup C_1 \cup C_{c-6}, k-1)\big]\\
&- \big[\underline{m(C_2 \cup C_2 \cup C_{c-7}, k-1)} + m(P_3 \cup C_1 \cup C_{c-7}, k-2)\big]\\
\overset{\text{lemma 5}}{=}\ & \big[\underline{m(P_5 \cup C_2 \cup C_{c-6}, k)} + m(C_1 \cup C_1 \cup C_2 \cup C_{c-6}, k-1)\big]\\
&+ \big[\underline{m(C_2 \cup C_1 \cup C_{c-6}, k-1)} + m(C_1 \cup C_1 \cup C_{c-6}, k-2)\big]\\
&+ m(C_2 \cup C_1 \cup C_{c-7}, k-2) - \big[\underline{m(P_5 \cup C_2 \cup C_{c-6}, k)}\\
&+ m(C_2 \cup C_2 \cup C_{c-6}, k-1)\big] - \underline{m(C_2 \cup C_1 \cup C_{c-6}, k-1)}\\
&- m(P_3 \cup C_1 \cup C_{c-7}, k-2)\\
\overset{\text{lemma 5}}{=}\ & \underline{m(C_1 \cup C_1 \cup C_2 \cup C_{c-6}, k-1)} + m(C_1 \cup C_1 \cup C_{c-6}, k-2)\\
&+ \big[\underline{m(P_3 \cup C_1 \cup C_{c-7}, k-2)} + m(C_1 \cup C_1 \cup C_{c-7}, k-3)\big]\\
&- \big[\underline{m(C_1 \cup C_1 \cup C_2 \cup C_{c-6}, k-1)} + m(C_2 \cup C_{c-6}, k-2)\big]\\
&- \underline{m(P_3 \cup C_1 \cup C_{c-7}, k-2)}\\
\overset{\text{lemma 5}}{=}\ & \underline{m(C_1 \cup C_1 \cup C_{c-6}, k-2)} + m(C_1 \cup C_1 \cup C_{c-7}, k-3)\\
&- \big[\underline{m(C_1 \cup C_1 \cup C_{c-6}, k-2)} + m(C_{c-6}, k-3)\big]\\
\overset{\text{lemma 5}}{=}\ & \big[\underline{m(C_1 \cup C_{c-7}, k-3)} + m(C_1 \cup C_{c-7}, k-4)\big]\\
&- \big[\underline{m(C_1 \cup C_{c-7}, k-3)} + m(C_{c-8}, k-4)\big]\\
\overset{\text{lemma 5}}{=}\ & \big[m(C_{c-7}, k-4) + m(C_{c-7}, k-5)\big] - m(C_{c-8}, k-4)\\
\overset{\text{lemma 5}}{=}\ & \big[m(C_1 \cup C_{c-8}, k-4) + m(C_{c-9}, k-5)\big] + m(C_{c-7}, k-5)\\
&- m(C_{c-8}, k-4)\\
\overset{\text{lemma 5}}{=}\ & \big[\underline{m(C_{c-8}, k-4)} + m(C_{c-8}, k-5)\big] + m(C_{c-9}, k-5)\\
&+ m(C_{c-7}, k-5) - \underline{m(C_{c-8}, k-4)} \geqslant 0,
\end{aligned}
$$

where $m(C_{c-9}, k-5) = 0$ if $c = 8$, and at each step the underlined terms are canceled out. When $k = 5$, the final inequality is sharp. $\square$

We proceed to give other total orderings.

Theorem 8.

(1) $T^c_{i,1}(a) \prec T^c_{i,3}(a) \prec \cdots \prec \cdots \prec T^c_{i,4}(a) \prec T^c_{i,2}(a)$, and

(2) $T^c_{1,j}(a) \prec T^c_{3,j}(a) \prec \cdots \prec \cdots \prec T^c_{4,j}(a) \prec T^c_{2,j}(a)$.

The orderings are similar to those of theorem 4. See the explanation after that theorem.

The proof calls for more preparation.

Lemma 9.

(1) $$\left|m\left(J^c_a, s\right) - m\left(J^c_{a-2}, s\right)\right| \geqslant \left|m\left(J^c_{a+1}, s\right) - m\left(J^c_{a-1}, s\right)\right|, \quad 1 \leqslant a \leqslant q-1,\ s \in Z. \tag{8}$$

When $s = a - 1$, the inequality is sharp.

(2) $$\left|m\left(J^c_q, s\right) - m\left(J^c_{q-2}, s\right)\right| \geqslant \left|m\left(J^c_q, s\right) - m\left(J^c_{q-1}, s\right)\right|, \quad c \equiv 1(2),\ s \in Z. \tag{9}$$

When $s = q - 1$, the inequality is sharp.

Proof. (1) By (6),

$$\begin{aligned}
&\left|m\left(J^c_a, s\right) - m\left(J^c_{a-2}, s\right)\right| \\
&\quad = m(P_{c-2a+1}, s-a+1) = m(P_{c-2a}, s-a+1) + m(P_{c-2a-1}, s-a) \\
&\quad = m(P_{c-2a}, s-a+1) + \left|m\left(J^c_{a+1}, s\right) - m\left(J^c_{a-1}, s\right)\right| \\
&\quad \geqslant \left|m\left(J^c_{a+1}, s\right) - m\left(J^c_{a-1}, s\right)\right|, \quad 1 \leqslant a \leqslant q-1,\ s \in Z.
\end{aligned}$$

When $s = a - 1$, the inequality is sharp.

(2) By (6) and (7),

$$\begin{aligned}
&\left|m\left(J^c_q, s\right) - m\left(J^c_{q-2}, s\right)\right| - \left|m\left(J^c_q, s\right) - m\left(J^c_{q-1}, s\right)\right| \\
&\quad = m(P_{c-2q+1}, s-q+1) - m(P_{c-2q}, s-q) \\
&\quad = \begin{cases} -1, & s = q,\ c \equiv 0(2), \\ 1, & s = q-1, \\ 0, & \text{otherwise}, \end{cases} \\
&\quad \geqslant 0, \quad c \equiv 1(2).
\end{aligned}$$

And when $s = q - 1$, the inequality is sharp. $\square$

Lemma 10. Let

$$\gamma^c(a, s) = m(P_{a-1} \cup P_{c-a+1}, s) + m(P_a \cup P_{c-a}, s), \quad 0 \leqslant a \leqslant \left\lfloor \frac{c+1}{2} \right\rfloor = r,\ c \geqslant 0,\ s \in Z.$$

Then

$$\gamma^c(0,s) \leqslant \gamma^c(2,s) \leqslant \cdots \leqslant \cdots \leqslant \gamma^c(3,s) \leqslant \gamma^c(1,s),$$

and for each of the inequalities, there is an s to make it sharp.

The ordering is similar to those of theorem 4 but in the inverse direction. See the explanation after that theorem.

Proof. Case 1: $c \equiv 0(2)$. In this case, $r = \lfloor (c+1)/2 \rfloor = \lfloor c/2 \rfloor = q$. By (8) and theorem 4 we have that, if $a \equiv 1(2)$,

$$\begin{aligned}\gamma^c(a,s) - \gamma^c(a-1,s) &= m\left(J_a^c, s\right) - m\left(J_{a-2}^c, s\right) \geqslant m\left(J_{a-1}^c, s\right) - m\left(J_{a+1}^c, s\right)\\ &= \gamma^c(a,s) - \gamma^c(a+1,s) \geqslant 0.\end{aligned}$$

Hence

$$\begin{aligned}&\gamma^c(a+1,s) - \gamma^c(a-1,s) = \left[\gamma^c(a,s) - \gamma^c(a-1,s)\right] - \left[\gamma^c(a,s) - \gamma^c(a+1,s)\right] \geqslant 0,\\ &\quad 1 \leqslant a \leqslant \left\lfloor \frac{c}{2} \right\rfloor - 1 = q - 1 = r - 1,\ s \in Z,\end{aligned}$$

and when $s = a - 1$, the inequality is sharp.

If $a \equiv 0(2)$,

$$\begin{aligned}\gamma^c(a-1,s) - \gamma^c(a,s) &= m\left(J_{a-2}^c, s\right) - m\left(J_a^c, s\right) \geqslant m\left(J_{a+1}^c, s\right) - m\left(J_{a-1}^c, s\right)\\ &= \gamma^c(a+1,s) - \gamma^c(a,s) \geqslant 0.\end{aligned}$$

Again,

$$\begin{aligned}&\gamma^c(a-1,s) - \gamma^c(a+1,s) = \left[\gamma^c(a-1,s) - \gamma^c(a,s)\right] - \left[\gamma^c(a+1,s) - \gamma^c(a,s)\right] \geqslant 0,\\ &\quad 1 \leqslant a \leqslant \left\lfloor \frac{c}{2} \right\rfloor - 1 = q - 1,\ s \in Z,\end{aligned}$$

and when $s = a - 1$, the inequality is sharp. In addition,

$$\gamma^c(r,s) - \gamma^c(r-1,s) = m\left(J_r^c, s\right) - m\left(J_{r-2}^c, s\right) \leqslant 0\ (\geqslant 0), \quad r \equiv 0(2)\ \left(r \equiv 1(2)\right),$$

and by (6), $s = r - 1$ gives sharp inequalities.

Case 2: $c \equiv 1(2)$. In this case, $r = q + 1$, $c = r + r - 1$, $\gamma^c(r,s) = m(J_{r-1}^c, s) + m(J_{r-1}^c, s)$. By (7),

$$\begin{aligned}\gamma^c(r,s) - \gamma^c(r-1,s) &= m\left(J_{r-1}^c, s\right) - m\left(J_{r-2}^c, s\right) = m\left(J_q^c, s\right) - \left(J_{q-1}^c, s\right)\\ &\geqslant 0\ (\leqslant 0), \quad r \equiv 1(2)\ \left(r \equiv 0(2)\right).\end{aligned}$$

When $s = q = r - 1$, the inequality is sharp.

By (9), if $r \equiv 0(2)$,

$$\begin{aligned}\gamma^c(r,s)-\gamma^c(r-2,s) &= \bigl[\gamma^c(r-1,s)-\gamma^c(r-2,s)\bigr]-\bigl[\gamma^c(r-1,s)-\gamma^c(r,s)\bigr]\\ &= m\bigl(J_q^c,s\bigr)-m\bigl(J_{q-2}^c,s\bigr)-\bigl[m\bigl(J_{q-1}^c,s\bigr)-m\bigl(J_q^c,s\bigr)\bigr]\\ &\geqslant 0, \quad s\in Z,\end{aligned}$$

and when $s = q-1$, the inequality is sharp. If $r \equiv 1(2)$, by (9),

$$\begin{aligned}\gamma^c(r-2,s)-\gamma^c(r,s) &= \bigl[\gamma^c(r-2,s)-\gamma^c(r-1,s)\bigr]-\bigl[\gamma^c(r,s)-\gamma^c(r-1,s)\bigr]\\ &= m\bigl(J_{q-2}^c,s\bigr)-m\bigl(J_q^c,s\bigr)-\bigl[m\bigl(J_q^c,s\bigr)-m\bigl(J_{q-1}^c,s\bigr)\bigr]\\ &\geqslant 0, \quad s\in Z,\end{aligned}$$

and when $s = q-1$, the inequality is sharp. The rest of the argument is the same as in case 1. □

Proof of theorem 8. Clearly, $m(\widehat{T}_{i,j}^c(a),s) = m(\widehat{T}_{k,l}^c(a),s)$. On the other hand,

$$\begin{aligned}\beta_1\bigl(\widehat{T}_{i,j}^c(a),s\bigr) &= \sum_{\delta+\lambda=s-2}\bigl[m(P_{i-2}\cup P_{a-i},\delta)+m(P_{i-1}\cup P_{a-i-1},\delta)\bigr]\\ &\qquad\times\bigl[m(P_{j-2}\cup P_{b-j},\lambda)+m(P_{j-1}\cup P_{b-j-1},\lambda)\bigr]\\ &= \sum_{\delta+\lambda=s-2}\gamma^{a-2}(i-1,\delta)\gamma^{b-2}(j-1,\lambda), \quad s\in Z. \qquad (10)\end{aligned}$$

By lemma 10, we have

$$\beta_1\bigl(\widehat{T}_{i,1}^c(a),s\bigr)\leqslant\beta_1\bigl(\widehat{T}_{i,3}^c(a),s\bigr)\leqslant\cdots\leqslant\cdots\leqslant\beta_1\bigl(\widehat{T}_{i,4}^c(a),s\bigr)\leqslant\beta_1\bigl(\widehat{T}_{i,2}^c(a),s\bigr)$$

and

$$\beta_1\bigl(\widehat{T}_{1,j}^c(a),s\bigr)\leqslant\beta_1\bigl(\widehat{T}_{3,j}^c(a),s\bigr)\leqslant\cdots\leqslant\cdots\leqslant\beta_1\bigl(\widehat{T}_{4,j}^c(a),s\bigr)\leqslant\beta_1\bigl(\widehat{T}_{2,j}^c(a),s\bigr).$$

Thus, by lemma 2, we get

$$T_{i,1}^c(a)\preceq T_{i,3}^c(a)\preceq\cdots\preceq\cdots\preceq T_{i,4}^c(a)\preceq T_{i,2}^c(a)$$

and

$$T_{1,j}^c(a)\preceq T_{3,j}^c(a)\preceq\cdots\preceq\cdots\preceq T_{4,j}^c(a)\preceq T_{2,j}^c(a).$$

The sharpness of the strict quasiorderings is derived from the fact that in (10), there is at least one term satisfying the strict inequality relation with its corresponding term for different i or j, which is guaranteed also by lemma 10. For instance,

$$\begin{aligned}&\gamma^{a-2}(i-1,0)\gamma^{b-2}(j-1,\lambda)>\gamma^{a-2}(i-1,0)\gamma^{b-2}(j-3,\lambda),\\ &\quad\text{if } \lambda=j-3\equiv 0(2),\end{aligned}$$

which ensures

$$\beta_1\bigl(\widehat{T}^c_{i,j}(a), j-1\bigr) > \beta_1\bigl(\widehat{T}^c_{i,j-2}(a), j-1\bigr), \quad \text{if } j \equiv 1(2).$$

Thus, by lemma 2, $T^c_{i,j}(a) \succ T^c_{i,j-2}(a)$, $j \equiv 1(2)$. □

Theorem 11. Suppose $5 \leqslant a < b$. Then

$$T^c_{1,3}(a) \succ T^c_{3,1}(a), \quad a \equiv 1(2),$$

or

$$T^c_{1,3}(a) \prec T^c_{3,1}(a), \quad a \equiv 0(2).$$

Proof. By (10),

$$\beta_1\bigl(\widehat{T}^c_{1,3}(a), s\bigr) = \sum_{\delta+\lambda=s-2} \gamma^{a-2}(0,\delta)\gamma^{b-2}(2,\lambda),$$
$$\beta_1\bigl(\widehat{T}^c_{3,1}(a), s\bigr) = \sum_{\delta+\lambda=s-2} \gamma^{a-2}(2,\delta)\gamma^{b-2}(0,\lambda),$$

$$\begin{aligned}
&\beta_1\bigl(\widehat{T}^c_{1,3}(a), s\bigr) - \beta_1\bigl(\widehat{T}^c_{3,1}(a), s\bigr)\\
&\quad= \sum_{\delta+\lambda=s-2} \bigl[\gamma^{a-2}(0,\delta)\gamma^{b-2}(2,\lambda) - \gamma^{a-2}(2,\delta)\gamma^{b-2}(0,\lambda)\bigr]\\
&\quad= \sum_{\delta+\lambda=s-2} \bigl[\gamma^{a-2}(0,\delta)\bigl(\gamma^{b-2}(2,\lambda) - \gamma^{b-2}(0,\lambda)\bigr)\\
&\qquad - \bigl(\gamma^{a-2}(2,\delta) - \gamma^{a-2}(0,\delta)\bigr)\gamma^{b-2}(0,\lambda)\bigr].
\end{aligned}$$

But

$$\begin{aligned}
\gamma^{b-2}(2,\lambda) - \gamma^{b-2}(0,\lambda) &= \bigl[\gamma^{b-2}(1,\lambda) - \gamma^{b-2}(0,\lambda)\bigr] - \bigl[\gamma^{b-2}(1,\lambda) - \gamma^{b-2}(2,\lambda)\bigr]\\
&= m\bigl(J_1^{b-2},\lambda\bigr) - \bigl[m\bigl(J_0^{b-2},\lambda\bigr) - m\bigl(J_2^{b-2},\lambda\bigr)\bigr]\\
&= m(P_{b-3},\lambda) - m(P_{b-5},\lambda-1) \quad \bigl(\text{by (6)}\bigr)\\
&= m(P_{b-4},\lambda). \qquad (11)
\end{aligned}$$

Likewise,

$$\begin{aligned}
\gamma^{a-2}(2,\delta) - \gamma^{a-2}(0,\delta) &= \begin{cases} 1, & \delta = 0,\ a = 5,\\ 0, & \delta \neq 0,\ a = 5,\\ m(P_{a-4},\delta), & a > 5, \end{cases}\\
&= m(P_{a-4},\delta). \qquad (12)
\end{aligned}$$

Substituting them into the above equations, we get

$$\begin{aligned}
&\beta_1\bigl(\widehat{T}^c_{1,3}(a), s\bigr) - \beta_1\bigl(\widehat{T}^c_{3,1}(a), s\bigr)\\
&\quad= \sum_{\delta+\lambda=s-2} \bigl[\gamma^{a-2}(0,\delta)m(P_{b-4},\lambda) - m(P_{a-4},\delta)\gamma^{b-2}(0,\delta)\bigr]
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{\delta+\lambda=s-2} \bigl[m(P_{a-2},\delta)m(P_{b-4},\delta) - m(P_{a-4},\delta)m(P_{b-2},\lambda)\bigr] \\
&= m(P_{a-2}\cup P_{b-4}, s-2) - m\bigl(J_{a-4}^{c-6}, s-2\bigr) \\
&= \begin{cases} m(J_{a-2}^{c-6}, s-2) - m(J_{a-4}^{c-6}, s-2), & b \geqslant a+2, \\ m(J_{a-3}^{c-6}, s-2) - m(J_{a-4}^{c-6}, s-2), & b = a+1, \end{cases} \\
&\begin{cases} \leqslant 0, & a \equiv 0(2), \\ \geqslant 0, & a \equiv 1(2), \end{cases} \quad \text{by (6) and (7).}
\end{aligned}
$$

And there obviously exists an s for each inequality to be sharp. The theorem holds by lemma 2. □

Theorem 12. When $b > a = 4$, $T_{1,3}^c(4) \prec T_{2,1}^c(4)$.

Proof. By (10),

$$
\begin{aligned}
\beta_1\bigl(\widehat{T}_{1,3}^c(4), s\bigr) &= \sum_{\delta+\lambda=s-2} \gamma^2(0,\delta)\gamma^{b-2}(2,\lambda), \\
\beta_1\bigl(\widehat{T}_{2,1}^c(4), s\bigr) &= \sum_{\delta+\lambda=s-2} \gamma^2(1,\delta)\gamma^{b-2}(0,\lambda).
\end{aligned}
$$

By (11) and (12),

$$
\begin{aligned}
&\beta_1\bigl(\widehat{T}_{1,3}^c(4), s\bigr) - \beta_1\bigl(\widehat{T}_{2,1}^c(4), s\bigr) \\
&\quad= \sum_{\delta+\lambda=s-2} \bigl[\gamma^2(0,\delta)\gamma^{b-2}(2,\lambda) - \gamma^2(1,\delta)\gamma^{b-2}(0,\lambda)\bigr] \\
&\quad= \sum_{\delta+\lambda=s-2} \bigl[\gamma^2(0,\delta)\bigl(\gamma^{b-2}(2,\lambda) - \gamma^{b-2}(0,\lambda)\bigr) - \bigl(\gamma^2(1,\delta) - \gamma^2(0,\delta)\bigr)\gamma^{b-2}(0,\lambda)\bigr] \\
&\quad= \sum_{\delta+\lambda=s-2} \bigl[\gamma^2(0,\delta)m(P_{b-4},\lambda) - m\bigl(J_1^2,\delta\bigr)m\bigl(J_0^{b-2},\lambda\bigr)\bigr] \\
&\quad= \sum_{\delta+\lambda=s-2} m(P_2,\delta)m(P_{b-4},\lambda) - \sum_{\delta+\lambda=s-2} m(P_1\cup P_1,\delta)m(P_{b-2},\lambda) \\
&\quad= \begin{cases} m(J_2^{b-2}, s-2) - m(J_0^{b-2}, s-2), & b \geqslant 6, \\ m(J_1^3, s-2) - m(J_0^3, s-2), & b = 5, \end{cases} \\
&\quad\leqslant 0.
\end{aligned}
$$

When $s = 3$, the inequality is sharp. □

Theorem 13. When $b > a = 3$, $T_{2,l}^c(3) \succ T_{1,j}^c(3)$, $1 \leqslant j, l \leqslant \lfloor (b+1)/2 \rfloor$.

Proof.

$$
\begin{aligned}
\beta_1\big(\widehat{T}^c_{2,l}(3),s\big) &= \sum_{\delta+\lambda=s-2} \gamma^1(1,\delta)\gamma^{b-2}(l-1,\lambda)\\
&= \sum_{\delta+\lambda=s-2} \big[m(P_1\cup P_0,\delta)+m(P_1\cup P_0,\delta)\big]\gamma^{b-2}(l-1,\lambda)\\
&\geqslant \sum_{\delta+\lambda=s-2} \big[m(P_1,\delta)+m(P_1,\delta)\big]\gamma^{b-2}(0,\lambda)\\
&= \sum_{\delta+\lambda=s-2} \big[m(P_1,\delta)+m(P_1,\delta)\big]m\big(J_0^{b-2},\lambda\big)\\
&\geqslant \sum_{\delta+\lambda=s-2} m\big(J_0^1,\delta\big)\big[m\big(J_0^{b-2},\lambda\big)+m\big(J_1^{b-2},\lambda\big)\big]\\
&= \sum_{\delta+\lambda=s-2} \gamma^1(0,\delta)\gamma^{b-2}(1,\lambda) \geqslant \sum_{\delta+\lambda=s-2} \gamma^1(0,\delta)\gamma^{b-2}(j-1,\lambda)\\
&= \beta_1\big(\widehat{T}^c_{1,j}(3),s\big).
\end{aligned}
$$

And there is at least an s that makes one of the above inequalities sharp. Thus, by lemma 2, $T^c_{2,l} \succ T^c_{1,j}(3)$. □

Theorem 14. Suppose $c \geqslant 10$, then $T^c_{1,i}(3) \prec T^c_{3,1}(5)$, $3 \leqslant i \leqslant \lfloor (c-2)/2 \rfloor$.

Proof. First of all, $J_3^c \prec J_5^c$. Then

$$
\begin{aligned}
\beta_1\big(\widehat{T}^c_{1,i}(3),s\big) &= \sum_{\delta+\lambda=s-2} \gamma^1(0,\delta)\gamma^{c-5}(i-1,\lambda) = \gamma^{c-5}(i-1,s-2)\\
&= m(P_{i-1}\cup P_{c-i-4},s-2) + m(P_{i-2}\cup P_{c-i-3},s-2)\\
&\overset{\text{lemma 6}}{=} \big[m(P_{c-6},s-2)+m(P_{i-3}\cup P_{c-i-6},s-4)\big]\\
&\quad + \big[m(P_{c-6},s-2)+m(P_{i-4}\cup P_{c-i-5},s-4)\big],
\end{aligned}
$$

$$
\begin{aligned}
\beta_1\big(\widehat{T}^c_{3,1}(5),s\big) &= \sum_{\delta+\lambda=s-2} \gamma^3(2,\delta)\gamma^{b-2}(0,\lambda)\\
&= \sum_{\delta+\lambda=s-2} \big[m(P_1\cup P_2,\delta)+m(P_1\cup P_2,\delta)\big]m(P_0\cup P_{b-2},\lambda)\\
&= \sum_{\delta+\lambda=s-2} \big[m(P_2,\delta)m(P_{b-2},\lambda)+m(P_2,\delta)m(P_{b-2},\lambda)\big]\\
&= m(P_2\cup P_{b-2},s-2)+m(P_2\cup P_{b-2},s-2)\\
&= m(P_2\cup P_{c-7},s-2)+m(P_2\cup P_{c-7},s-2)\\
&\overset{\text{lemma 6}}{=} \big[m(P_{c-6},s-2)+m(P_{c-9},s-4)\big]
\end{aligned}
$$

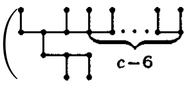
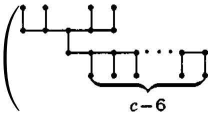
$$
\begin{aligned}
&+ \big[m(P_{c-6}, s-2) + m(P_{c-9}, s-4)\big] \\
\geqslant\ & \beta_1\big(\widehat{T}^c_{1,i}(3), s\big).
\end{aligned}
$$

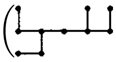
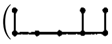
By lemma 2, $T^c_{1,i}(3) \prec T^c_{3,1}(5)$. □

Theorem 15. Under the same condition as in the previous theorem, $T^c_{1,2}(3) \succ T^c_{3,1}(5)$.

Proof.

$m\big(T^c_{1,2}(3), k\big) - \big(T^c_{3,1}(5), k\big)$

$= m\Big($  $, k\Big) - m\Big($  $, k\Big)$

$\overset{\text{lemma 5}}{=} m\Big($  $\cup C_{c-6}, k\Big) + m\big($  $\cup C_{c-7}, k-1\big)$

$\quad - m(C_5 \cup C_{c-6}, k) - m\big($  $\cup C_{c-7}, k-1\big)$

$\overset{\text{lemma 5}}{=} \big[\underline{m(C_3 \cup C_2 \cup C_{c-6}, k)} + m(P_5 \cup C_1 \cup C_{c-6}, k-1)\big]$

$\quad + \big[m(C_2 \cup C_2 \cup C_{c-7}, k-1) + m(P_3 \cup C_1 \cup C_{c-7}, k-2)\big]$

$\quad - \big[\underline{m(C_3 \cup C_2 \cup C_{c-6}, k)} + m(C_2 \cup C_1 \cup C_{c-6}, k-1)\big]$

$\quad - \big[m\big($  $\cup C_2 \cup C_{c-7}, k-1\big) + m(C_2 \cup C_1 \cup C_{c-7}, k-2)\big]$

$$
\begin{aligned}
\overset{\text{lemma 5}}{=}\ & \big[\underline{m(C_2 \cup C_1 \cup C_{c-6}, k-1)} + m(P_3 \cup C_1 \cup C_{c-6}, k-2)\big] \\
& + \underline{m(C_2 \cup C_2 \cup C_{c-7}, k-1)} + \underline{m(P_3 \cup C_1 \cup C_{c-7}, k-2)} \\
& - \underline{m(C_1 \cup C_2 \cup C_{c-6}, k-1)} \\
& - \big[\underline{(C_2 \cup C_2 \cup C_{c-7}, k-1)} + m(C_2 \cup C_1 \cup C_{c-7}, k-2)\big] \\
& - \big[\underline{m(P_3 \cup C_1 \cup C_{c-7}, k-2)} + m(C_1 \cup C_1 \cup C_{c-7}, k-3)\big] \\
\overset{\text{lemma 5}}{=}\ & \big[m(P_3 \cup C_1 \cup C_1 \cup C_{c-7}, k-2) + m(P_3 \cup C_1 \cup C_{c-8}, k-3)\big] \\
& - \big[m(C_1 \cup C_1 \cup C_1 \cup C_{c-7}, k-2) + m(C_1 \cup C_{c-7}, k-3)\big] \\
& - m(C_1 \cup C_1 \cup C_{c-7}, k-7) \\
\overset{\text{lemma 5}}{=}\ & \big[\underline{m(C_1 \cup C_1 \cup C_1 \cup C_{c-7}, k-2)} + \underline{m(C_1 \cup C_1 \cup C_{c-7}, k-3)}\big] \\
& + m(P_3 \cup C_1 \cup C_{c-8}, k-3) - \underline{m(C_1 \cup C_1 \cup C_1 \cup C_{c-7}, k-2)} \\
& - m(C_1 \cup C_{c-7}, k-3) - \underline{m(C_1 \cup C_1 \cup C_{c-7}, k-3)} \\
\overset{\text{lemma 6}}{=}\ & \big[\underline{m(C_1 \cup C_{c-7}, k-3)} + m(C_1 \cup C_{c-9}, k-5) + m(C_1 \cup C_{c-10}, k-5)\big] \\
& - \underline{m(C_1 \cup C_{c-7}, k-3)} \\
=\ & m(C_1 \cup C_{c-9}, k-5) + m(C_1 \cup C_{c-10}, k-5) \geqslant 0.
\end{aligned}
$$

In the above equations the underlined terms at each step are canceled out. When $k = 5$, we get the strict inequality. □

Theorem 16. Suppose $c \geqslant 14$, then $T^c_{3,1}(5) \prec T^c_{3,1}(2t+1),\ t \geqslant 3$.

Proof. By theorem 4, $J^c_5 \prec J^c_{2t+1}$.

$$\begin{aligned}
\beta_1\big(\widehat{T}^c_{3,1}(5), s\big) &= m(P_2 \cup P_{c-7}, s-2) + m(P_2 \cup P_{c-7}, s-2) \\
&\overset{\text{lemma 6}}{=} \big[m(P_{c-6}, s-2) + m(P_{c-9}, s-4)\big] + m(P_2 \cup P_{c-7}, s-2) \\
&\overset{\text{lemma 5}}{=} \underline{m(P_{c-6}, s-2)} + \big[\underline{m(P_{2t-4} \cup P_{c-2t-5}, s-4)} \\
&\quad + \underline{m(P_{2t-5} \cup P_{c-2t-6}, s-5)}\big] + \underline{m(P_2 \cup P_{c-7}, s-2)},
\end{aligned}$$

$$\begin{aligned}
\beta_1\big(\widehat{T}^c_{3,1}(2t+1), s\big) &= \sum_{\delta+\lambda=s-2} \gamma^{2t-1}(2,\delta)\gamma^{c-2t-3}(0,\lambda) \\
&= \sum_{\delta+\lambda=s-2} \big[m(P_1 \cup P_{2t-2}, \delta) \\
&\quad + m(P_2 \cup P_{2t-3}, \delta)\big] m(P_{c-2t-3}, \lambda) \\
&= m(P_{2t-2} \cup P_{c-2t-3}, s-2) \\
&\quad + m(P_2 \cup P_{2t-3} \cup P_{c-2t-3}, s-2) \\
&\overset{\text{lemma 6}}{=} \big[m(P_{c-6}, s-2) + m(P_{2t-4} \cup P_{c-2t-5}, s-4) \\
&\quad + m(P_2 \cup P_{2t-3} \cup P_{c-2t-3}, s-2)\big] \\
&\overset{\text{lemma 6}}{=} m(P_{c-6}, s-2) + m(P_{2t-4} \cup P_{c-2t-5}, s-4) \\
&\quad + \big[m(P_2 \cup P_{c-7}, s-2) + m(P_2 \cup P_{2t-5} \cup P_{c-2t-5}, s-4)\big] \\
&\overset{\text{lemma 5}}{=} m(P_{c-6}, s-2) + m(P_{2t-4} \cup P_{c-2t-5}, s-4) \\
&\quad + m(P_2 \cup P_{c-7}, s-2) + \big[m(P_{2t-5} \cup P_{c-2t-5}, s-4) \\
&\quad + m(P_{2t-5} \cup P_{c-2t-5}, s-5)\big] \\
&\overset{\text{lemma 5}}{=} \underline{m(P_{c-6}, s-2)} + \underline{m(P_{2t-4} \cup P_{c-2t-5}, s-4)} \\
&\quad + \underline{m(P_2 \cup P_{c-7}, s-2)} + m(P_{2t-5} \cup P_{c-2t-5}, s-4) \\
&\quad + \big[\underline{m(P_{2t-5} \cup P_{c-2t-6}, s-5)} \\
&\quad + m(P_{2t-5} \cup P_{c-2t-7}, s-6)\big].
\end{aligned}$$

$$\begin{aligned}
&\beta_1\big(\widehat{T}^c_{3,1}(2t+1), s\big) - \beta_1\big(\widehat{T}^c_{3,1}(5), s\big) \\
&\quad = m(P_{2t-5} \cup P_{c-2t-5}, s-4) + m(P_{2t-5} \cup P_{c-2t-7}, s-6) \geqslant 0.
\end{aligned}$$

As a result of lemma 2, $T^c_{3,1}(5) \prec T^c_{3,1}(2t+1)$. □

Theorem 17. When $c \geqslant 10$, $T^c_{1,3}(5) \prec T^c_{1,3}(2t),\ t \geqslant 1$.

Proof. By theorem 4, $J_5^c \prec J_{2t}^c$.

$$\begin{aligned}\beta_1\big(\widehat{T}_{1,3}^c(5), s\big) &= \sum_{\delta+\lambda=s-2} \gamma^3(0,\delta)\gamma^{b-2}(2,\lambda)\\ &= \sum_{\delta+\lambda=s-2} m(P_3,\delta)\big[m(P_1\cup P_{c-8},\lambda)+m(P_2\cup P_{c-9},\lambda)\big]\\ &= m(P_3\cup P_{c-8}, s-2)+m(P_3\cup P_2\cup P_{c-9}, s-2),\end{aligned}$$

and likewise,

$$\beta_1\big(\widehat{T}_{1,3}^c(2t), s\big) = m(P_{2t-2}\cup P_{c-2t-3}, s-2)+m(P_{2t-2}\cup P_2\cup P_{c-2t-4}, s-2).$$

Because $2t \leqslant c/2$, we have $t \leqslant c/4$. And if $2t-2 > c-2t-3$ or $2t-2 > c-2t-4$, it implies $4t \leqslant c < 4t+1$ or $4t+2$, which holds only when $c \geqslant 12$.

Case 1: $10 \leqslant c < 12$. In this case, $t \leqslant c/4 < 3$, $2t-2 \leqslant c-2t-3$, and $2t-2 \leqslant c-2t-4$, by the above argument. Thus

$$\begin{aligned}\beta_1\big(\widehat{T}_{1,3}^c(2t), s\big) &= m(P_{2t-2}\cup P_{c-2t-3}, s-2)+m(P_{2t-2}\cup P_2\cup P_{c-2t-4}, s-2)\\ &= m\big(J_{2t-2}^{c-5}, s-2\big)+m\big(P_2\cup J_{2t-2}^{c-6}, s-2\big)\\ &\geqslant m(P_3\cup P_{c-8}, s-2)+m(P_2\cup P_3\cup P_{c-9}, s-2)\\ &\qquad (c-8, c-9 > 0,\ 2t-2 \leqslant 2)\\ &= \beta_1\big(\widehat{T}_{1,3}^c(5), s\big).\end{aligned}$$

Case 2: $c \geqslant 12$. In this case,

$$\begin{aligned}\beta_1\big(\widehat{T}_{1,3}^c(5), s\big) &= m(P_3\cup P_{c-8}, s-2)+m(P_3\cup P_2\cup P_{c-9}, s-2)\\ &= m\big(J_3^{c-5}, s-2\big)+m\big(J_3^{c-6}\cup P_2, s-2\big) \quad (c-8,\ c-9 \geqslant 3)\\ &\leqslant m(P_{2t-2}\cup P_{c-2t-3}, s-2)+m(P_2\cup P_{2t-2}\cup P_{c-2t-4}, s-2)\\ &= \beta_1\big(\widehat{T}_{1,3}^c(2t), s\big),\end{aligned}$$

for $c-2t \geqslant 12-2t \geqslant 12-(c-2t)$ implies $c-2t \geqslant 6$; hence $c-2t-3 > c-2t-4 \geqslant 2$, while $P_{2t-2}\cup P_{c-2t-3}$ is either J_{2t-2}^{c-5} or J_{c-2t-3}^{c-5}, and $P_{2t-2}\cup P_{c-2t-4}$ is either J_{2t-2}^{c-6} or J_{c-2t-4}^{c-6}. $\square$

Summing the above theorems up, the reader can deduce that $T_{3,1}^c(5)$ has the smallest energy among trees of two-component capped graphs after $T_{1,1}^c(i)$, $1 \leqslant i \leqslant \lfloor c/2\rfloor$ and $T_{1,j}^c(3)$, $3 \leqslant j \leqslant \lfloor (c-2)/2\rfloor$.

4. The multi-component capped graphs and central results

Theorem 18. Suppose $n \geqslant 18$. If $c(\widehat{T}) \geqslant 3$, then

$$T \succ T_{3,1}^c(5), \quad c = \frac{n}{2}+1.$$

Proof. Concatenate $\widehat{T}$ into $\widehat{T}^*$ so that $c(\widehat{T}^*) = 3$ if $c(\widehat{T}) > 3$. It is feasible because $\widehat{T}$ together with the linking edges E forms a "tree structure" if we regard the paths as vertices. And the tree structure has at least two pendant "vertices". If we concatenate the two "vertices", paths of $\widehat{T}$ actually, the number of the connected components decreases. By lemma 3, $T \succ T^*$. Without loss of generality, we just consider $\widehat{T}$ with 3 connected components.

Suppose $\widehat{T} = P_f \cup P_g \cup P_h$, $f, g, h \geqslant 2$, $f+g+h = n/2+2 = c+1$. And let $P_f = u_1u_2 \cdots u_f$, $P_g = v_1v_2 \cdots v_g$, $P_h = w_1w_2 \cdots w_h$, and $T = T(\widehat{T}, \{u_iv_j, v_kw_l\})$, $1 \leqslant i \leqslant \lfloor (f+1)/2 \rfloor$, $1 \leqslant j < k \leqslant g$, $j \leqslant g-k+1$, $1 \leqslant l \leqslant \lfloor (h+1)/2 \rfloor$.

Case 1: One of i, j, l is not 1, or $k \neq g$, that is, one of i, j, k, l is the subscript of an inner vertex of P_f, P_g, P_h. Without loss of generality, we say j is an inner vertex of P_g.

(i) $g > \lfloor c/2 \rfloor$. Then $f \leqslant \lfloor c/2 \rfloor$. If $f \neq 3$, by lemma 3,

$$\begin{aligned} T &\succ T(P_f \cup P_{g+h-1}, u_iv_j) = T(P_f \cup P_{c-f}, u_iv_j) \succeq T(P_f \cup P_{c-f}, u_1v_j) \\ &= T^c_{1,j}(f) \succeq T^c_{1,3}(f) \quad (j \neq 1) \\ &\begin{cases} \succeq T^c_{3,1}(f) \succeq T^c_{3,1}(5), & f \equiv 1(2) \quad \text{(theorems 11, 16)}, \\ \succ T^c_{1,3}(5) \succeq T^c_{3,1}(5), & f \equiv 0(2) \quad \text{(theorem 17)}. \end{cases} \end{aligned}$$

If $f = 3$, then $(3 \neq f+h-1 \leqslant \lfloor c/2 \rfloor)$

$$\begin{aligned} T &\succ T(P_g \cup P_{f+h-1}, u_iv_j) = T(P_{f+h-1} \cup P_{c-f-h+1}, u_iv_j) \\ &\succeq T(P_{f+h-1} \cup P_{c-f-h+1}, u_1v_j) \succeq T(P_{f+h-1} \cup P_{c-f-h+1}, u_1v_3) \\ &= T^c_{1,3}(f+h-1) \\ &\begin{cases} \succeq T^c_{3,1}(f+h-1) \succeq T^c_{3,1}(5), & f+h-1 \equiv 1(2) \quad \text{(theorems 11, 16)}, \\ \succ T^c_{1,3}(5) \succeq T^c_{3,1}(5), & f+h-1 \equiv 0(2) \quad \text{(theorem 17)}. \end{cases} \end{aligned}$$

(ii) $g \leqslant \lfloor c/2 \rfloor$. Then, if $g \geqslant 5$,

$$\begin{aligned} T &\succ T(P_{f+h-1} \cup P_g, u_iv_j) = T(P_g \cup P_{c-g}, v_ju_i) = T^c_{j,i}(g) \succeq T^c_{j,1}(g) \succeq T^c_{3,1}(g) \\ &\begin{cases} \succeq T^c_{1,3}(g) \succ T^c_{1,3}(5) \succeq T^c_{3,1}(5), & g \equiv 0(2) \quad \text{(theorems 11, 17)}, \\ \succeq T^c_{3,1}(5), & g \equiv 1(2) \quad \text{(theorem 16)}. \end{cases} \end{aligned}$$

If $g = 4$, then

$$\begin{aligned} T &\succ T(P_{f+h-1} \cup P_g, u_iv_j) = T(P_g \cup P_{c-g}, v_ju_i) = T^c_{j,i}(g) \succeq T^c_{j,1}(g) \\ &= T^c_{2,1}(4) \succ T^c_{1,3}(4) \succ T^c_{1,3}(5) \succeq T^c_{3,1}(5) \quad \text{(theorems 11, 12, 17)}. \end{aligned}$$

If $g = 3$, then $j = 2$:

$$\begin{aligned} T &\succ T(P_g \cup P_{c-g}, v_ju_i) = T^c_{j,i}(g) \succeq T^c_{j,1}(g) = T^c_{2,1}(g) = T^c_{2,1}(3) \succ T^c_{1,2}(3) \\ &\succ T^c_{3,1}(5) \quad \text{(theorem 15)}. \end{aligned}$$

Case 2: $i = j = l = 1$, $k = g$. To begin with, we compare $m(\widehat{T}, s)$ and $m(\widehat{T}^c_{3,1}(5), s)$:

$$m\big(\widehat{T}^c_{3,1}(5), s\big) = m(P_5 \cup P_{c-5}, s) = m\big(J^c_5, s\big).$$

For $\widehat{T}$, there are at least two of f, g, h which are no more than $\lfloor c/2 \rfloor$, say f and g. If one of them, say f, is not three, then

$$m\big(\widehat{T}, s\big) = m(P_f \cup P_g \cup P_h, s) \geqslant m(P_f \cup P_{g+h-1}, s) \geqslant m(P_5 \cup P_{c-5}, s) = m\big(\widehat{T}^c_{3,1}(5), s\big).$$

If $f = g = 3$, then

$$m\big(\widehat{T}, s\big) \geqslant m(P_{f+g-1} \cup P_h, s) = m(P_5 \cup P_{c-5}, s) = m\big(\widehat{T}^c_{3,1}(5), s\big).$$

In any case, $m(\widehat{T}, s) \geqslant m(\widehat{T}^c_{3,1}(5), s)$ and $m(\widehat{T}, 2) > m(\widehat{T}^c_{3,1}(5), 2)$. Next we compare $\beta_1(\widehat{T}, s)$ and $\beta_1(\widehat{T}^c_{3,1}(5), s)$:

$$\begin{aligned}
\beta_1\big(\widehat{T}^c_{3,1}(5), s\big) &= m(P_2 \cup P_{c-7}, s-2) + m(P_2 \cup P_{c-7}, s-2),\\
\beta_1\big(\widehat{T}, s\big) &= m(P_{f-2} \cup P_{c-f-2}, s-2) + m(P_{c-h-2} \cup P_{h-2}, s-2)\\
&\geqslant m(P_{c-5}, s-2) + m(P_{c-5}, s-2)\\
&= m\big(J^{c-5}_0, s-2\big) + m\big(J^{c-5}_0, s-2\big)\\
&\geqslant m\big(J^{c-5}_2, s-2\big) + m\big(J^{c-5}_2, s-2\big)\\
&= m(P_2 \cup P_{c-7}, s-2) + m(P_2 \cup P_{c-7}, s-2)\\
&= \beta_1\big(\widehat{T}^c_{3,1}(5), s\big).
\end{aligned}$$

When $s = 3$, i.e., $s - 2 = 2 - 1$, by (6), $m(J^{c-5}_0, s-2) > m(J^{c-5}_2, s-2)$; hence $\beta_1(\widehat{T}, s) > \beta_1(\widehat{T}^c_{3,1}(5), s)$. By lemma 2, $T \succ T^c_{3,1}(5)$. $\square$

In summary, we have the following central result.

Theorem 19. For $c \geqslant 10$,

$$\begin{aligned}
T^c_{1,1}(1) &\prec T^c_{1,1}(3) \prec \cdots \prec \cdots \prec \cdots \prec T^c_{1,1}(4) \prec T^c_{1,1}(2)\\
&\prec T^c_{1,3}(3) \prec T^c_{1,5}(3) \prec \cdots \prec \cdots \prec \cdots \prec T^c_{1,6}(3) \prec T^c_{1,4}(3)\\
&\prec T^c_{3,1}(5) \prec T,
\end{aligned}$$

where T is any tree in Ψ_n not in the previous series.

For this ordering please refer to the explanation after theorem 4.

Consequently, we get altogether $2\lfloor (1/2)(n/2+1) \rfloor - 2$ or, roughly, $n/2 - 1$ trees preceding the rest in the class Ψ_n in the increasing order of their energies.

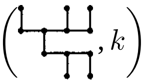
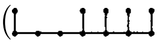
5. Complementations

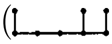
The last theorem in section 3 has the restriction of $c \geqslant 10$. Now we will complement the theorem to the extent of $c \geqslant 7$, that is, $n \geqslant 12$. For the case $n \leqslant 10$, there are existent total orderings. We note that essentially the restriction applies only to theorems 7, 14, 15, 17 and 18. The following theorems correspond to these theorems, respectively, for the cases of $c = 7, 8, 9$.

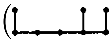
Theorem 20. $T^7_{1,1}(2) \prec T^7_{1,2}(3)$.

Proof. The difference of the numbers of the k-matchings is

$m\big(T^7_{1,2}(3), k\big) - m\big(T^7_{1,1}(2), k\big)$

$= m\Big($  $, k\Big) - m\big($  $, k\big)$

$= m\big($  $\cup C_2, k\big) + m\big($  $\cup C_1 \cup C_1, k-1\big)$

$\quad - m\big($  $\cup C_2, k\big) - m(P_6 \cup C_1, k-1)$

$= m\big($  $\cup C_1 \cup C_1, k-1\big) - m(P_6 \cup C_1, k-1)$

$$
\begin{aligned}
&= \big[\underline{m(C_2 \cup C_1 \cup C_1, k-1)} + m(C_1 \cup C_1 \cup C_1, k-2)\big]\\
&\quad - \big[\underline{m(C_2 \cup C_1 \cup C_1, k-1)} + m(P_3 \cup C_1, k-2)\big]\\
&= m(C_1 \cup C_1 \cup C_1, k-2) - m(P_3 \cup C_1, k-2)\\
&\overset{\text{lemma 6}}{=} \big[\underline{m(P_3 \cup C_1, k-2)} + m(C_1, k-4)\big] - \underline{m(P_3 \cup C_1, k-2)}\\
&= m(C_1, k-4) \geqslant 0.
\end{aligned}
$$

When $k = 4$, the inequality is sharp. □

Theorem 21. $T^9_{1,3}(3) \prec T^9_{1,3}(4)$, $T^8_{1,3}(3) \prec T^8_{1,2}(3) \prec T^8_{1,2}(4)$, $T^7_{1,2}(3) \prec T^7_{1,3}(2)$.

Proof. Theorem 4 implies that $\beta_0(\widehat{T}^9_{1,3}(3), s) < \beta_0(\widehat{T}^9_{1,3}(4), s)$, $\beta_0(\widehat{T}^8_{1,2}(3), s) < \beta_0(\widehat{T}^8_{1,2}(4), s)$, and $\beta_0(\widehat{T}^7_{1,2}(3), s) < \beta_0(\widehat{T}^7_{1,3}(2), s)$. On the other hand,

$$
\begin{aligned}
&\beta_1\big(\widehat{T}^9_{1,3}(4), s\big) - \beta_1\big(\widehat{T}^9_{1,3}(3), s\big)\\
&\quad = \big[\underline{m(C_1 \cup C_1, s-2)} + m(C_1 \cup C_1, s-2)\big]\\
&\qquad - \big[m(P_3, s-2) + \underline{m(C_1 \cup C_1, s-2)}\big]\\
&\quad = m(C_1 \cup C_1, s-2) - m(P_3, s-2)\\
&\quad \overset{\text{lemma 6}}{=} \big[m(P_3, s-2) + m(\emptyset, s-4)\big] - m(P_3, s-2) = m(\emptyset, s-4) \geqslant 0,
\end{aligned}
$$

$$
\begin{aligned}
&\beta_1\big(\widehat{T}^8_{1,2}(4), s\big) - \beta_1\big(\widehat{T}^8_{1,2}(3), s\big)\\
&\quad = \big[m(C_1 \cup C_1, s-2) + \underline{m(C_1, s-2)}\big] - \big[m(P_3, s-2) + \underline{m(C_1, s-2)}\big]
\end{aligned}
$$

$$
\begin{aligned}
&= m(C_1 \cup C_1, s-2) - m(P_3, s-2)\\
&\overset{\text{lemma 6}}{=} \bigl[m(P_3, s-2) + m(\emptyset, s-4)\bigr] - m(P_3, s-2) = m(\emptyset, s-4) \geqslant 0,
\end{aligned}
$$

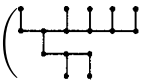
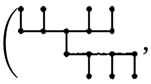
$$
\begin{aligned}
&\beta_1\bigl(\widehat{T}^7_{1,3}(2), s\bigr) - \beta_1\bigl(\widehat{T}^7_{1,2}(3), s\bigr)\\
&\quad = \underline{2m(C_1, s-2)} - \bigl[\underline{m(C_1, s-2)} + m(\emptyset, s-2)\bigr]\\
&\quad = m(C_1, s-2) - m(\emptyset, s-2) \geqslant 0.
\end{aligned}
$$

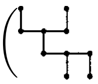
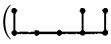
By lemma 2, we are done. $\square$

Theorem 22. $T^9_{1,3}(4) \prec T^9_{1,2}(3)$.

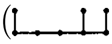
Proof. For we have

$m\bigl(T^9_{1,2}(3), k\bigr) - m\bigl(T^9_{1,3}(4), k\bigr)$

$= m\Bigl($  $, k\Bigr) - m\Bigl($  $, k\Bigr)$

$= m\Bigl($  $\cup C_3, k\Bigr) + m\bigl($  $\cup C_2, k-1\bigr)$

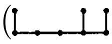
$\quad - m(C_5 \cup C_3, k) - m\bigl($  $\cup C_2, k-1\bigr)$

$= \bigl[m\bigl($  $\cup C_3, k\bigr) + m\bigl($  $\cup C_3, k-1\bigr)\bigr]$

$\quad + \bigl[m(C_2 \cup C_2 \cup C_2, k-1) + m(P_3 \cup C_1 \cup C_2, k-2)\bigr]$

$\quad - \bigl[m\bigl($  $\cup C_3, k\bigr) + m(C_2 \cup C_2 \cup C_3, k-1)\bigr]$

$\quad - \bigl[m\bigl($  $\cup C_2 \cup C_2, k-1\bigr) + m(C_1 \cup C_2 \cup C_2, k-2)\bigr]$

$= m\bigl($  $\cup C_3, k-1\bigr) + m(C_2 \cup C_2 \cup C_2, k-1)$

$\quad + m(P_3 \cup C_1 \cup C_2, k-2) - m(C_2 \cup C_2 \cup C_3, k-1)$

$\quad - m\bigl($  $\cup C_2 \cup C_2, k-1\bigr) - m(C_1 \cup C_2 \cup C_2, k-2)$

$$
\begin{aligned}
&= \bigl[\underline{m(C_2 \cup C_2 \cup C_3, k-1)} + m(P_3 \cup C_1 \cup C_3, k-2)\bigr]\\
&\quad + \underline{m(C_2 \cup C_2 \cup C_2, k-1)} + m(P_3 \cup C_1 \cup C_2, k-2)\\
&\quad - \underline{m(C_2 \cup C_2 \cup C_3, k-1)} - \bigl[\underline{m(C_2 \cup C_2 \cup C_2, k-1)}\\
&\quad + m(C_1 \cup C_2 \cup C_2, k-2)\bigr] - m(C_1 \cup C_2 \cup C_2, k-2)\\
&= m(P_3 \cup C_1 \cup C_3, k-2) + m(P_3 \cup C_1 \cup C_2, k-2)\\
&\quad - m(C_1 \cup C_2 \cup C_2, k-2) - m(C_1 \cup C_2 \cup C_2, k-2)\\
&= \bigl[m(P_3 \cup C_1 \cup C_1 \cup C_2, k-2) + m(P_3 \cup C_1 \cup C_1, k-3)\bigr]\\
&\quad + m(P_3 \cup C_1 \cup C_2, k-2) - m(C_1 \cup C_2 \cup C_2, k-2)\\
&\quad - \bigl[m(C_1 \cup P_3 \cup C_2, k-2) + m(C_1 \cup C_1 \cup C_2, k-3)\bigr]
\end{aligned}
$$

$$\begin{aligned}
&\overset{\text{lemma 6}}{=} \big[\underline{m(C_2 \cup C_1 \cup C_2, k-2)} + m(C_2 \cup C_1, k-4)\big] \\
&\quad + \underline{m(P_3 \cup C_1 \cup C_1, k-3)} + \underline{m(P_3 \cup C_1 \cup C_2, k-2)} \\
&\quad - \underline{m(C_1 \cup C_2 \cup C_2, k-2)} - \underline{m(C_1 \cup P_3 \cup C_2, k-2)} \\
&\quad - \big[\underline{m(C_1 \cup C_1 \cup P_3, k-3)} + m(C_1 \cup C_1 \cup C_1, k-4)\big] \\
&= m(C_2 \cup C_1, k-4) - m(C_1 \cup C_1 \cup C_1, k-4) \\
&= \big[\underline{m(C_1 \cup C_1 \cup C_1, k-4)} + m(C_1, k-5)\big] - \underline{m(C_1 \cup C_1 \cup C_1, k-4)} \\
&= m(C_1, k-5) \geqslant 0.
\end{aligned}$$

When $k = 5$, the inequality is sharp. □

Theorem 23. $T^9_{1,3}(4) \prec T^9_{1,3}(2)$, $T^8_{1,2}(4) \prec T^8_{1,3}(2)$.

Proof. By theorem 4, $\beta_0(\widehat{T}^9_{1,3}(4), s) < \beta_0(\widehat{T}^9_{1,3}(2), s)$ and $\beta_0(\widehat{T}^8_{1,2}(4), s) < \beta_0(\widehat{T}^8_{1,3}(2), s)$. In addition,

$$\begin{aligned}
&\beta_1\big(\widehat{T}^9_{1,3}(2), s\big) - \beta_1\big(\widehat{T}^9_{1,3}(4), s\big) \\
&\quad = \big[m(P_4, s-2) + m(P_2 \cup P_3, s-2)\big] - 2m(P_2 \cup P_2, s-2) \\
&\quad = \big[\underline{m(P_2 \cup P_2, s-2)} + m(P_1 \cup P_1, s-3)\big] + \big[\underline{m(P_2 \cup P_2, s-2)} \\
&\qquad + m(P_2 \cup P_1, s-3)\big] - \underline{2m(P_2 \cup P_2, s-2)} \\
&\quad = m(\emptyset, s-3) + m(P_2, s-3) \geqslant 0,
\end{aligned}$$

$$\begin{aligned}
&\beta_1\big(\widehat{T}^8_{1,3}(2), s\big) - \beta_1\big(\widehat{T}^8_{1,2}(4), s\big) \\
&\quad = \big[m(P_3, s-2) + \underline{m(P_2 \cup P_2, s-2)}\big] - \big[\underline{m(P_2 \cup P_2, s-2)} + m(P_2, s-2)\big] \\
&\quad = m(P_3, s-2) - m(P_2, s-2) \geqslant 0.
\end{aligned}$$

By lemma 2, we are done. □

Theorem 24. If $c(\widehat{T}) \geqslant 3$, then $T \succ T^9_{1,3}(4)$ $(c = 9)$, $T \succ T^8_{1,2}(3)$ $(c = 8)$, $T \succ T^7_{1,2}(3)$ $(c = 7)$.

Proof. Case 1: One of i, j, k is not 1, or $k \neq g$. Without loss of generality, we say j is an inner vertex of P_g.

(i) $g > \lfloor c/2 \rfloor$. Then, if $f \neq 3$, by theorem 23,

$$T \succ T(P_f \cup P_{g+h-1}, u_i v_j) = T^c_{i,j}(f) \succeq T^c_{1,j}(f) \succeq \begin{cases} T^c_{1,3}(4), & c = 9, \\ T^c_{1,2}(4) \succ T^8_{1,2}(3), & c = 8, \\ T^c_{1,3}(2) \succeq T^7_{1,2}(3), & c = 7. \end{cases}$$

If $f = 3$, then $f + h - 1 \neq 3$; hence

$$T \succ T(P_{f+h-1} \cup P_{c-(g+h-1),u_i v_j}) \succeq \begin{cases} T^c_{1,3}(4), & c = 9, \\ T^c_{1,2}(4) \succ T^8_{1,2}(3), & c = 8, \\ T^c_{1,3}(2) \succeq T^7_{1,2}(3), & c = 7. \end{cases}$$

(ii) $g \leqslant \lfloor c/2 \rfloor$. In this case, $g = 3, 4$, $j = 2$. If $g = 4$, by theorem 12 (in the case $c = 9$),

$$\begin{aligned} T &\succ T(P_{f+h-1} \cup P_g, u_i v_j) = T(P_g \cup P_{c-g}, v_j u_i) = T^c_{j,i}(4) \succeq T^c_{j,1}(4) \\ &\succeq \begin{cases} T^c_{1,3}(4), & c = 9, \\ T^c_{1,2}(4) \succ T^8_{1,2}(3), & c = 8. \end{cases} \end{aligned}$$

If $g = 3$, then by theorem 22 ($c = 9$),

$$T \succ T(P_g \cup P_{c-g}, v_j u_i) \succeq T^c_{2,1}(g) = T^c_{2,1}(3) \succ \begin{cases} T^c_{1,2}(3) \succ T^c_{1,3}(4), & c = 9, \\ T^c_{1,2}(3), & c = 8, \\ T^c_{1,2}(3), & c = 7. \end{cases}$$

Case 2: $i = j = l = 1$, $k = g$. For $\widehat{T}$, there are at least two of f, g, h which do not exceed $\lfloor c/2 \rfloor$, say f and g. If one of them, say f, is not three, then

$$\widehat{T} = P_f \cup P_g \cup P_h \succ P_f \cup P_{g+h-1} = J^c_f \succeq \begin{cases} J^c_4, & c = 9, \\ J^c_3, & c = 8, \\ J^c_2, & c = 7. \end{cases}$$

If $f = g = 3$, then

$$\widehat{T} = P_f \cup P_g \cup P_h \succ P_{f+g-1} \cup P_h = P_5 \cup P_h = \begin{cases} J^c_4, & c = 9, \\ J^c_3, & c = 8, \\ J^c_2, & c = 7. \end{cases}$$

On the other hand,

$$\begin{aligned} \beta_1\big(\widehat{T}, s\big) &= m(P_{f-2} \cup P_{c-f-2}, s-2) + m(P_{c-h-2} \cup P_{h-2}, s-2) \\ &\geqslant 2m(P_{c-5}, s-2) \geqslant \begin{cases} \beta_1\big(\widehat{T}^c_{1,3}(4), s\big), & c = 9, \\ \beta_1\big(\widehat{T}^c_{1,2}(3), s\big), & c = 8, \\ \beta_1\big(\widehat{T}^c_{1,3}(2), s\big), & c = 7. \end{cases} \end{aligned}$$

Hence, by lemma 2,

$$T \succ \begin{cases} T^c_{1,3}(4), & c = 9, \\ T^c_{1,2}(3) \succ T^8_{1,2}(3), & c = 8, \\ T^c_{1,3}(2) \succ T^7_{1,2}(3), & c = 7. \end{cases} \qquad \square$$

In the final analysis, we get

Theorem 25.

$$T^7_{1,1}(1) \prec T^7_{1,1}(3) \prec T^7_{1,1}(2) \prec T^7_{1,2}(3) \prec T,$$
$$T^8_{1,1}(1) \prec T^8_{1,1}(3) \prec T^8_{1,1}(4) \prec T^8_{1,1}(2) \prec T^8_{1,3}(3) \prec T^8_{1,2}(3) \prec T,$$
$$T^9_{1,1}(1) \prec T^9_{1,1}(3) \prec T^9_{1,1}(4) \prec T^9_{1,1}(2) \prec T^9_{1,3}(3) \prec T^9_{1,3}(4) \prec T.$$

Remark. Another tree has been added to the series in theorem 19, that is,

Theorem 26. For $c \geqslant 11$ ($n \geqslant 20$),

$$\begin{aligned} T^c_{1,1}(1) &\prec T^c_{1,1}(3) \prec \cdots \prec \cdots \prec \cdots \prec T^c_{1,1}(4) \prec T^c_{1,1}(2) \\ &\prec T^c_{1,3}(3) \prec T^c_{1,5}(3) \prec \cdots \prec \cdots \prec \cdots \prec T^c_{1,6}(3) \prec T^c_{1,4}(3) \\ &\prec T^c_{3,1}(5) \prec T^c_{1,3}(5) \prec T, \end{aligned}$$

where T is any tree in $\boldsymbol{\Psi}_n$ not in the previous series.

And

Theorem 27.

$$T^7_{1,1}(1) \prec T^7_{1,1}(3) \prec T^7_{1,1}(2) \prec T^7_{1,2}(3) \prec T^7_{2,1}(3) \prec T^7_{1,3}(2) \prec T,$$
$$T^8_{1,1}(1) \prec T^8_{1,1}(3) \prec T^8_{1,1}(4) \prec T^8_{1,1}(2) \prec T^8_{1,3}(3) \prec T^8_{1,2}(3) \prec T^8_{1,2}(4) \prec T,$$
$$T^9_{1,1}(1) \prec T^9_{1,1}(3) \prec T^9_{1,1}(4) \prec T^9_{1,1}(2) \prec T^9_{1,3}(3) \prec T^9_{1,3}(4) \prec T^9_{1,2}(3) \prec T,$$
$$\begin{aligned} T^{10}_{1,1}(1) &\prec T^{10}_{1,1}(3) \prec T^{10}_{1,1}(5) \prec T^{10}_{1,1}(4) \prec T^{10}_{1,1}(2) \prec T^{10}_{1,3}(3) \prec T^{10}_{1,4}(3) \prec T^{10}_{3,1}(5) \\ &\prec T^{10}_{1,3}(4) \prec T. \end{aligned}$$

On balance, we get altogether $2\lfloor (1/2)(n/2+1) \rfloor - 1$ or, roughly, $n/2$ trees preceding the rest in the class $\boldsymbol{\Psi}_n$ in the increasing order of their energies.

References

[1] D.M. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs – Theory and Application* (VEB Deutscher Verlag der Wissenschaften, Berlin, 1982) p. 60.

[2] I. Gutman, Acyclic systems with extremal Hückel π-electron energy, Theoret. Chim. Acta (Berlin) 45 (1977) 79–87.

[3] I. Gutman, Acyclic conjugated molecules, trees and their energies, J. Math. Chem. 1 (1987) 123–143.

[4] I. Gutman and O.E. Polansky, *Mathematical Concepts in Organic Chemistry* (Springer, Berlin, 1986) pp. 135–142.

[5] I. Gutman and F. Zhang, On the ordering of graphs with respect to their matching numbers, Discrete Appl. Math. 15 (1986) 25–33.

[6] I. Gutman and F. Zhang, On the quasiordering of bipartite graphs, Publ. Inst. Math. Nouv. Sér. 40(54) (1986) 11–15.

[7] Q. Li and K. Feng, Some results about the spectral properties of graphs, J. Univ. Sci. Technol. China (1979) 53–56.

[8] F. Zhang and Z. Lai, The totally ordered subset in a sort of Hasse graphs of trees, J. Xinjiang Univ. (1983) 12–20.

[9] F. Zhang and Z. Lai, Three theorems of comparison of trees by their energy, Sci. Exploration 3 (1983) 35–36.

[10] F. Zhang and H. Li, On acyclic conjugated molecules with minimal energies, Discrete Appl. Math. 92 (1999) 71–84.