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Extremal Graph with Respect to Matching Energy for a Random Polyphenyl Chain [1]

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Abstract

The energy of a graph G is equal to the sum of absolute values of its eigenvalues of G. The matching energy (ME) of a graph G is recently proposed by Gutman and Wagner and pointed out that its chemical applications go back to the 1970s. It is defined as the sum $\sum_{i=1}^{n} |\mu_i|$, where $\mu_1, \mu_2, \cdots, \mu_n$ are the zeros of matching polynomial of G. In this paper, we determine the extremal graph with respect to the number of k-matching and the matching energy for a random polyphenyl chain.

1 Introduction

In this paper, the graphs under our consideration are finite, connected, undirected and simple. Let $\lambda_1, \lambda_2, \cdots, \lambda_n$ be the eigenvalues of a graph G. The energy of graph G is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$ in [11]. A matching in a graph G is a set of pairwise nonadjacent edges. A matching M is called k-matching if the size of M is k. By $m(G, k)$ we denote the number of k-matchings (i.e., the number of selections of k independent edges) of G, where $m(G, 0) = 1$, $m(G, 1) = m$ and $m(G, k) = 0$ for $k > \frac{n}{2}$.

The matching polynomial of the graph G is defined as

$$\alpha(G) = \alpha(G, \lambda) = \sum_{k \geq 0} (-1)^k m(G, k) \lambda^{n-2k}$$

and its theory can be found in [4, 10, 12].

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An important result in the theory of graph energy is the Coulson-type integral formula [11]

$$E(T) = \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2}\ln[\sum_{k\geq 0} m(T,k)\lambda^{2k}]dx \tag{1}$$

valid for any forest T.

In fact, the right hand side of formula (1) is well defined for any graph. Gutman and Wagner [14] considered it also for cycle-containing graphs, and the quantity is called the matching energy $ME(G)$ of a graph G. It is defined as

$$ME(G) = \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2}\ln[\sum_{k\geq 0} m(G,k)\lambda^{2k}]dx \tag{2}$$

Knowing how formula (1) was obtained [3, 11, 13], it can straightforwardly be obtained that

$$ME(G) = \sum_{i=1}^{n} |\mu_i|$$

where $\mu_1, \mu_2, \cdots, \mu_n$ are the zeros of matching polynomial of G.

In theoretical chemistry, the simple relation $TRE(G) = E(G) - ME(G)$ shows that the matching energy is a quantity of relevance for chemical applications, where $E(G)$ is the energy and $TRE(G)$ denotes the topological resonance energy of the molecular graph G. The theory of graph energy is well developed nowadays, but the matching energy has been undertaken until Gutman and Wagner [14] determined its basic properties, recently. The present paper is aimed at determining extremal graphs with respect to the matching energy for random polyphenylene chains.

2 Preliminaries

Before proceeding, we introduce some further notation.

Polyphenyls and their derivatives, which can be used in organic synthesis, drug synthesis, heat exchangers, etc., attracted the attention of chemists for many years [5, 15, 16]. Some results on energy, Merrield-Simmons index, Hosoya index and Wiener index of the polyphenyl chains were reported in [1, 2, 9, 8, 18]. Recently, Deng [6, 7] gave the recurrences or explicit formulae for computing the Wiener index and Kirchhoff index of the polyphenyl chains. Yang and Zhang [17] obtain a simple exact formula for the expected value of the Wiener index of a random polyphenyl chain.

A polyphenyl chain PPC_n with n hexagons can be regarded as a polyphenyl chain PPC_{n-1} with $n-1$ hexagons to which a new terminal hexagon has been adjoined by a cut edge, see Figure 1.

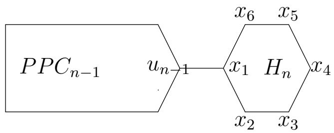

Figure 1: A polyphenyl chain PPC_n with n hexagons, $c_n = x_1$ and ortho-vertices $o_n = x_2, x_6$, meta-vertices $m_n = x_3, x_5$, and para-vertex $p_n = x_4$ in H_n.

Let $PPC_n = H_1H_2 \cdots H_n$ be a polyphenyl chain with $n(n \geq 2)$ hexagons, where H_k is the k-th hexagon of PPC_n attached to H_{k-1} by a cut edge $u_{k-1}c_k$, $k = 2, 3, \cdots, n$. A vertex v of H_k is said to be ortho-, meta- and para-vertex of H_k if the distance between v and c_k is 1, 2 and 3, denoted by o_k, m_k and p_k, respectively. Examples of ortho-, meta-, and para-vertices are shown in Figure 1. Except the first hexagon, any hexagon in a polyphenyl chain has two ortho-vertices, two meta-vertices and one para-vertex.

A polyphenyl chain PPC_n is a polyphenyl ortho-chain if $u_k = o_k$ for $2 \leq k \leq n-1$. A polyphenyl chain PPC_n is a polyphenyl meta-chain if $u_k = m_k$ for $2 \leq k \leq n-1$. A polyphenyl chain PPC_n is a polyphenyl para-chain if $u_k = p_k$ for $2 \leq k \leq n-1$. The polyphenyl ortho-, meta- and para-chain with n hexagons are denoted by O_n, M_n and L_n, respectively.

For $n \geq 3$, the terminal hexagon can be attached to meta-, ortho-, or para-vertex in three ways, which results in the local arrangements we describe as PPC^1_{n+1}, PPC^2_{n+1}, PPC^3_{n+1}, see Figure 2.

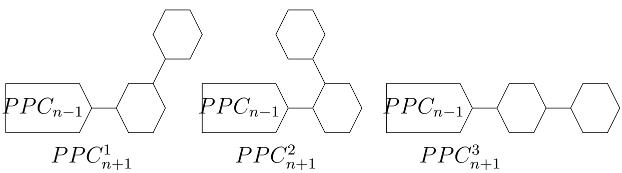

Figure 2: The three types of local arrangements in polyphenyl chains

A random polyphenyl chain $PPC(n, p_1, p_2)$ with n hexagons is a polyphenyl chain obtained by stepwise addition of terminal hexagons. At each step $k(= 3, 4, \cdots, n)$, a random selection is made from one of the three possible constructions:

(i)$PPC_{k-1} \to PPC^1_k$ with probability p_1,

(ii)$PPC_{k-1} \to PPC^2_k$ with probability p_2, (iii)$PPC_{k-1} \to PPC_k^3$ with probability $1 - p_1 - p_2$

where the probabilities p_1 and p_2 are constants, irrespective to the step parameter k.

Specially, the random polyphenyl chain $PPC(n, 1, 0)$ is the polyphenyl meta-chain M_n, $PPC(n, 0, 1)$ is the polyphenyl orth-chain O_n, and $PPC(n, 0, 0)$ is the polyphenyl para-chain L_n, respectively. The three types of uniform chains are shown in Figure 3.

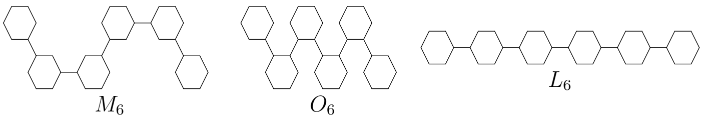

Figure 3. The three types of chains M_n, O_n and L_n.

For a random polyphenyl chain $PPC(n, p_1, p_2)$, the number of k-matching and the matching energy are random variables. In this paper, we will determine the extremal graphs with respect to the number of k-matching and the matching energy for a random polyphenylene chain, respectively.

The cut-vertex u of the rightmost hexagon and the cut-edge $e = uv$ incident to it will play special roles in our computations. We call them the critical vertex and the critical edge, respectively. Three auxiliary graphs that appear as components of G by deleting the edge e and the end vertices of e are shown in Figure 4. For a polyphenylene chain G_n, its auxiliary graph is denoted by G'_n, where G stands for O, M, or L.

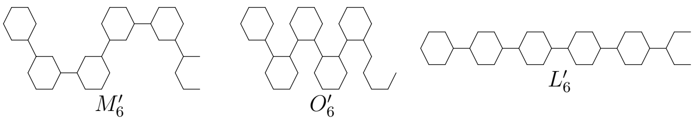

Figure 4. The three types of auxiliary graphs M'_n, O'_n and L'_n.

Analogously, three auxiliary graphs of a random polyphenyl chain $PPC(n, p_1, p_2)$ that appear as components of G by deleting e and the end vertices of e are shown in Figure 5. For a polyphenylene chain PPC_n, its auxiliary graph is denoted by PPC'_n.

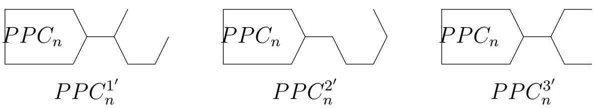

Figure 5. The three types of auxiliary graphs of a random polyphenyl chain.

3 The extremal graph with respect to the number of k-matching and the matching energy

The quasi-order $\succ$, defined by $G \succ H \Leftrightarrow m(G,k) \geq m(H,k)$ for all k, has proved fundamental in the study of the graph energy and the Hosoya index, but it is also interesting in its own right. From the definition of the matching energy, it is clear that $G \succ H$ implies $ME(G) \geq ME(H)$. Here, we will apply the important technique to the matching energy of a random polyphenyl chain.

The following results will be used in the computations.

Lemma 1. *[4] [12] (i) If uv is an edge of G, then $m(G,k) = m(G-uv,k) + m(G-u-v,k-1)$;*

(ii) If u is a vertex of G, then $m(G,k) = m(G-u,k) + \sum_{v \in N(u)} m(G-u-v,k-1)$, where $N(u)$ is the neighbours of u in G.

We can easily get the following lemma:

Lemma 2. *Let G_1, G_2, G_3 and G_4 be four graphs. If $m(G_1,i) \geq m(G_2,i)$ and $m(G_3,i) \geq m(G_4,i)$ for $i = 0,1,\cdots,k$, then $m(G_1 \cup G_3,k) \geq m(G_2 \cup G_4,k)$.*

Theorem 3. *Let PPC_n be a random polyphenyl chain of length n. Then for any $0 \leq k \leq 3n$,*

$$m(M_n,k) \leq m(PPC_n,k) \leq m(O_n,k)$$

where M_n and O_n are the meta-chain and the ortho-chain of length n, respectively.

Proof. We will proof the theorem by the mathematical induction.

It is easily to find the theorem is true for $n = 1$ or $n = 2$.

If $n = 3$, then

$$\begin{aligned} m(M_3,k) &= m(M_2 \cup C_6,k) + m(M_1' \cup P_5,k-1) \\ &= m(M_2 \cup C_6,k) + m(M_1 \cup 2P_5,k-1) + m(2P_5 \cup P_3,k-2) \end{aligned}$$

$$\begin{aligned} m(O_3,k) &= m(O_2 \cup C_6,k) + m(O_1' \cup P_5,k-1) \\ &= m(O_2 \cup C_6,k) + m(O_1 \cup 2P_5,k-1) + m(2P_5 \cup P_4,k-2) \end{aligned}$$

$$\begin{aligned} m(PPC_3,k) &= m(PPC_2 \cup C_6,k) + p_1 m(PPC_1^{1\prime} \cup P_5,k-1) \\ &+ p_2 m(PPC_1^{2\prime} \cup P_5,k-1) + p_3 m(PPC_1^{3\prime} \cup P_5,k-1) \\ &= m(PPC_2 \cup C_6,k) + m(PPC_1 \cup 2P_5,k-1) + p_1 m(2P_5 \cup P_3,k-2) \\ &+ p_2 m(2P_5 \cup P_4,k-2) + p_3 m(2P_5 \cup 2P_2,k-2) \end{aligned}$$

Using Lemma 2, we can easily get

$$m(2P_5 \cup P_3, k-2) \le m(2P_5 \cup 2P_2, k-2) \le m(2P_5 \cup P_4, k-2)$$

And

$$\begin{aligned} & m(2P_5 \cup P_3, k-2) \\ \le\ & p_1 m(2P_5 \cup P_3, k-2) + p_2 m(2P_5 \cup P_4, k-2) + p_3 m(2P_5 \cup 2P_2, k-2) \\ \le\ & m(2P_5 \cup P_4, k-2) \end{aligned}$$

Note that

$$m(M_2 \cup C_6, k) = m(PPC_2 \cup C_6, k) = m(O_2 \cup C_6, k)$$

$$m(M_1 \cup 2P_5, k-1) = m(PPC_1 \cup 2P_5, k-1) = m(O_1 \cup 2P_5, k-1)$$

we have $m(M_3, k) \le m(PPC_3, k) \le m(O_3, k)$.

Now, we assume that it is true for a random polyphenyl chain with the length less than n.

Let PPC_n be a random polyphenyl chain of length n. It is obvious that $m(M_n, k) \le m(PPC_n, k) \le m(O_n, k)$ for $k = 0, 1$.

If $2 \le k < n$, then

$$\begin{aligned} & m(M_n, k) \\ =\ & m(M_{n-1} \cup C_6, k) + m(M'_{n-2} \cup P_5, k-1) \\ =\ & m(M_{n-1} \cup C_6, k) + m(M_{n-2} \cup 2P_5, k-1) + m(M'_{n-3} \cup P_5 \cup P_3, k-2) \\ =\ & m(M_{n-1} \cup C_6, k) + m(M_{n-2} \cup 2P_5, k-1) + m(M_{n-3} \cup 2P_5 \cup P_3, k-2) \\ & + m(M'_{n-4} \cup P_5 \cup 2P_3, k-3) \\ =\ & \cdots \\ =\ & m(M_{n-1} \cup C_6, k) + m(M_{n-2} \cup 2P_5, k-1) + m(M_{n-3} \cup 2P_5 \cup P_3, k-2) \\ & + \cdots + m(M_{n-k} \cup 2P_5 \cup (k-2)P_3, 1) + m(M'_{n-k-1} \cup P_5 \cup (k-1)P_3, 0) \\ =\ & m(M_{n-1} \cup C_6, k) + m(M_{n-2} \cup 2P_5, k-1) + m(M_{n-3} \cup 2P_5 \cup P_3, k-2) \\ & + \cdots + m(M_{n-k} \cup 2P_5 \cup (k-2)P_3, 1) + 1 \\ =\ & m(M_{n-1} \cup C_6, k) + \sum_{t=0}^{k-2} m(M_{n-2-t} \cup 2P_5 \cup tP_3, k-1-t) + 1 \end{aligned}$$

$$\begin{aligned} & m(O_n, k) \\ =\ & m(O_{n-1} \cup C_6, k) + m(O'_{n-2} \cup P_5, k-1) \\ =\ & m(O_{n-1} \cup C_6, k) + m(O_{n-2} \cup 2P_5, k-1) + m(O'_{n-3} \cup P_5 \cup P_4, k-2) \\ =\ & m(O_{n-1} \cup C_6, k) + m(O_{n-2} \cup 2P_5, k-1) + m(O_{n-3} \cup 2P_5 \cup P_4, k-2) \\ & + m(O'_{n-4} \cup P_5 \cup 2P_4, k-3) \\ =\ & \cdots \\ =\ & m(O_{n-1} \cup C_6, k) + m(O_{n-2} \cup 2P_5, k-1) + m(O_{n-3} \cup 2P_5 \cup P_4, k-2) \\ & + \cdots + m(O_{n-k} \cup 2P_5 \cup (k-2)P_4, 1) + m(O'_{n-k-1} \cup P_5 \cup (k-1)P_4, 0) \\ =\ & m(O_{n-1} \cup C_6, k) + m(O_{n-2} \cup 2P_5, k-1) + m(O_{n-3} \cup 2P_5 \cup P_4, k-2) \\ & + \cdots + m(O_{n-k} \cup 2P_5 \cup (k-2)P_4, 1) + 1 \\ =\ & m(O_{n-1} \cup C_6, k) + \sum_{t=0}^{k-2} m(O_{n-2-t} \cup 2P_5 \cup tP_4, k-1-t) + 1 \end{aligned}$$

$$
\begin{aligned}
& m(PPC_n,k)\\
= \; & m(PPC_{n-1}\cup C_6,k)+p_1m(PPC^{1\prime}_{n-2}\cup P_5,k-1)+p_2m(PPC^{2\prime}_{n-2}\cup P_5)\\
& +p_3m(PPC^{3\prime}_{n-2}\cup P_5)\\
= \; & m(PPC_{n-1}\cup C_6,k)+m(PPC_{n-2}\cup 2P_5,k-1)+p_1[p_1m(PPC^{1\prime}_{n-3}\cup P_5\cup P_3,k-2)\\
& +p_2m(PPC^{2\prime}_{n-3}\cup P_5\cup P_3,k-2)+p_3m(PPC^{3\prime}_{n-3}\cup P_5\cup P_3,k-2)]\\
& +p_2[p_1m(PPC^{1\prime}_{n-3}\cup P_5\cup P_4,k-2)+p_2m(PPC^{2\prime}_{n-3}\cup P_5\cup P_4,k-2)\\
& +p_3m(PPC^{3\prime}_{n-3}\cup P_5\cup P_4,k-2)]+p_3[p_1m(PPC^{1\prime}_{n-3}\cup P_5\cup 2P_2,k-2)\\
& +p_2m(PPC^{2\prime}_{n-3}\cup P_5\cup 2P_2,k-2)+p_3m(PPC^{3\prime}_{n-3}\cup P_5\cup 2P_2,k-2)]\\
= \; & m(PPC_{n-1}\cup C_6,k)+m(PPC_{n-2}\cup 2P_5,k-1)\\
& +(p_1^2+p_1p_2+p_1p_3)m(PPC_{n-3}\cup 2P_5\cup P_3,k-2)\\
& +(p_1p_2+p_2^2+p_2p_3)m(PPC_{n-3}\cup 2P_5\cup P_4,k-2)\\
& +(p_1p_3+p_3p_2+p_3^2)m(PPC_{n-3}\cup 2P_5\cup 2P_2,k-2)\\
& +p_1^2[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup 2P_3,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup 2P_3,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup 2P_3,k-3)]\\
& +p_1p_2[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup P_4\cup P_3,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup P_4\cup P_3,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup P_4\cup P_3,k-3)]\\
& +p_1p_3[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup P_3\cup 2P_2,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup P_3\cup 2P_2,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup P_3\cup 2P_2,k-3)]\\
& +p_1p_2[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup P_4\cup P_3,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup P_4\cup P_3,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup P_4\cup P_3,k-3)]\\
& +p_2^2[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup 2P_4,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup 2P_4,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup 2P_4,k-3)]\\
& +p_2p_3[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup P_4\cup 2P_2,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup P_4\cup 2P_2,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup P_4\cup 2P_2,k-3)]\\
& +p_1p_3[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup P_3\cup 2P_2,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup P_3\cup 2P_2,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup P_3\cup 2P_2,k-3)]\\
& +p_2p_3[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup P_4\cup 2P_2,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup P_4\cup 2P_2,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup P_4\cup 2P_2,k-3)]\\
& +p_3^2[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup 4P_2,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup 4P_2,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup 4P_2,k-3)]\\
= \; & m(PPC_{n-1}\cup C_6,k)+m(PPC_{n-2}\cup 2P_5,k-1)+p_1m(PPC_{n-3}\cup 2P_5\cup P_3,k-2)\\
& +p_2m(PPC_{n-3}\cup 2P_5\cup P_4,k-2)+p_3m(PPC_{n-3}\cup 2P_5\cup 2P_2,k-2)\\
& +p_1^2[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup 2P_3,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup 2P_3,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup 2P_3,k-3)]\\
& +2p_1p_2[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup P_4\cup P_3,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup P_4\cup P_3,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup P_4\cup P_3,k-3)]\\
& +2p_1p_3[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup P_3\cup 2P_2,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup P_3\cup 2P_2,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup P_3\cup 2P_2,k-3)]\\
& +p_2^2[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup 2P_4,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup 2P_4,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup 2P_4,k-3)]\\
& +2p_2p_3[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup P_4\cup 2P_2,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup P_4\cup 2P_2,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup P_4\cup 2P_2,k-3)]\\
& +p_3^2[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup 4P_2,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup 4P_2,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup 4P_2,k-3)]\\
= \; & \cdots
\end{aligned}
$$

$$
\begin{aligned}
&= m(PPC_{n-1}\cup C_6,k)\\
&\quad +\sum_{t=0}^{k-2}\sum_{t_1+t_2+t_3=t}\tfrac{t!}{t_1!t_2!t_3!}p_1^{t_1}p_2^{t_2}p_3^{t_3}m(PPC_{n-2-t}\cup 2P_5\cup t_1P_3\cup t_2P_4\cup 2t_3P_2,k-1-t)+1
\end{aligned}
$$

If $n\le k\le 3n$, then

$$
\begin{aligned}
& m(M_n,k)\\
=\;& m(M_{n-1}\cup C_6,k)+m(M'_{n-2}\cup P_5,k-1)\\
=\;& m(M_{n-1}\cup C_6,k)+m(M_{n-2}\cup 2P_5,k-1)+m(M'_{n-3}\cup P_5\cup P_3,k-2)\\
=\;& m(M_{n-1}\cup C_6,k)+m(M_{n-2}\cup 2P_5,k-1)+m(M_{n-3}\cup 2P_5\cup P_3,k-2)\\
& +m(M'_{n-4}\cup P_5\cup 2P_3,k-3)\\
=\;& \cdots\\
=\;& m(M_{n-1}\cup C_6,k)+m(M_{n-2}\cup 2P_5,k-1)+\cdots\\
& +m(M_1\cup 2P_5\cup (n-3)P_3,k-n+2)+m(2P_5\cup (n-2)P_3,k-n+1)\\
=\;& m(M_{n-1}\cup C_6,k)+\sum_{t=0}^{n-2}m(M_{n-2-t}\cup 2P_5\cup tP_3,k-1-t)
\end{aligned}
$$

$$
\begin{aligned}
& m(O_n,k)\\
=\;& m(O_{n-1}\cup C_6,k)+m(O'_{n-2}\cup P_5,k-1)\\
=\;& m(O_{n-1}\cup C_6,k)+m(O_{n-2}\cup 2P_5,k-1)+m(O'_{n-3}\cup P_5\cup P_4,k-2)\\
=\;& m(O_{n-1}\cup C_6,k)+m(O_{n-2}\cup 2P_5,k-1)+m(O_{n-3}\cup 2P_5\cup P_3,k-2)\\
& +m(O'_{n-4}\cup P_5\cup 2P_4,k-3)\\
=\;& \cdots\\
=\;& m(O_{n-1}\cup C_6,k)+m(O_{n-2}\cup 2P_5,k-1)+\cdots\\
& +m(O_1\cup 2P_5\cup (n-3)P_4,k-n+2)+m(2P_5\cup (n-2)P_4,k-n+1)\\
=\;& m(O_{n-1}\cup C_6,k)+\sum_{t=0}^{n-2}m(O_{n-2-t}\cup 2P_5\cup tP_4,k-1-t)
\end{aligned}
$$

$$
\begin{aligned}
& m(PPC_n,k)\\
=\;& m(PPC_{n-1}\cup C_6,k)+p_1m(PPC^{1\prime}_{n-2}\cup P_5,k-1)\\
& +p_2m(PPC^{2\prime}_{n-2}\cup P_5,k-1)+p_3m(PPC^{3\prime}_{n-2}\cup P_5,k-1)\\
=\;& m(PPC_{n-1}\cup C_6,k)+m(PPC_{n-2}\cup 2P_5,k-1)\\
& +p_1[p_1m(PPC^{1\prime}_{n-3}\cup P_5\cup P_3,k-2)+p_2m(PPC^{2\prime}_{n-3}\cup P_5\cup P_3,k-2)\\
& +p_3m(PPC^{3\prime}_{n-3}\cup P_5\cup P_3,k-2)]\\
& +p_2[p_1m(PPC^{1\prime}_{n-3}\cup P_5\cup P_4,k-2)+p_2m(PPC^{2\prime}_{n-3}\cup P_5\cup P_4,k-2)\\
& +p_3m(PPC^{3\prime}_{n-3}\cup P_5\cup P_4,k-2)]\\
& +p_3[p_1m(PPC^{1\prime}_{n-3}\cup P_5\cup 2P_2,k-2)+p_2m(PPC^{2\prime}_{n-3}\cup P_5\cup 2P_2,k-2)\\
& +p_3m(PPC^{3\prime}_{n-3}\cup P_5\cup 2P_2,k-2)]\\
=\;& m(PPC_{n-1}\cup C_6,k)+m(PPC_{n-2}\cup 2P_5,k-1)\\
& +(p_1^2+p_1p_2+p_1p_3)m(PPC_{n-3}\cup 2P_5\cup P_3,k-2)\\
& +(p_1p_2+p_2^2+p_2p_3)m(PPC_{n-3}\cup 2P_5\cup P_4,k-2)\\
& +(p_1p_3+p_3p_2+p_3^2)m(PPC_{n-3}\cup 2P_5\cup 2P_2,k-2)\\
& +p_1^2[p_1m(PPC^{1\prime}_{n-4}\cup P_5\cup 2P_3,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup 2P_3,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup 2P_3,k-3)]\\
& +p_1p_2[P_1m(PPC^{1\prime}_{n-4}\cup P_5\cup P_3\cup P_4,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup P_3\cup P_4,k-3)\\
& +p_3m(PPC^{3\prime}_{n-4}\cup P_5\cup P_3\cup P_4,k-3)]\\
& +p_1p_3[P_1m(PPC^{1\prime}_{n-4}\cup P_5\cup P_3\cup 2P_2,k-3)+p_2m(PPC^{2\prime}_{n-4}\cup P_5\cup P_3\cup 2P_2,k-3)
\end{aligned}
$$

$$
\begin{aligned}
& +p_3m(PPC^{3\prime}_{n-4} \cup P_5 \cup P_3 \cup 2P_2, k-3)] \\
& +p_1p_2[p_1m(PPC^{1\prime}_{n-4} \cup P_5 \cup P_4 \cup P_3, k-3) + p_2m(PPC^{2\prime}_{n-4} \cup P_5 \cup P_4 \cup P_3, k-3) \\
& +p_3m(PPC^{3\prime}_{n-4} \cup P_5 \cup P_4 \cup P_3, k-3)] \\
& +p_2^2[p_1m(PPC^{1\prime}_{n-4} \cup P_5 \cup 2P_4, k-3) + p_2m(PPC^{2\prime}_{n-4} \cup P_5 \cup 2P_4, k-3) \\
& +p_3m(PPC^{3\prime}_{n-4} \cup P_5 \cup 2P_4, k-3)] \\
& +p_2p_3[p_1m(PPC^{1\prime}_{n-4} \cup P_5 \cup P_4 \cup 2P_2, k-3) + p_2m(PPC^{2\prime}_{n-4} \cup P_5 \cup P_4 \cup 2P_2, k-3) \\
& +p_3m(PPC^{3\prime}_{n-4} \cup P_5 \cup P_4 \cup 2P_2, k-3)] \\
& +p_1p_3[p_1m(PPC^{1\prime}_{n-4} \cup P_5 \cup 2P_2 \cup p_3, k-3) + p_2m(PPC^{2\prime}_{n-4} \cup P_5 \cup 2P_2 \cup P_3, k-3) \\
& +p_3m(PPC^{3\prime}_{n-4} \cup P_5 \cup 2P_2 \cup P_3, k-3)] \\
& +p_2p_3[p_1m(PPC^{1\prime}_{n-4} \cup P_5 \cup 2P_2 \cup P_4, k-3) + p_2m(PPC^{2\prime}_{n-4} \cup P_5 \cup 2P_2 \cup P_4, k-3) \\
& +p_3m(PPC^{3\prime}_{n-4} \cup P_5 \cup 2P_2 \cup P_4, k-3)] \\
& +p_3^2[p_1m(PPC^{1\prime}_{n-4} \cup P_5 \cup 4P_2, k-3) + p_2m(PPC^{2\prime}_{n-4} \cup P_5 \cup 4P_2, k-3) \\
& +p_3m(PPC^{3\prime}_{n-4} \cup P_5 \cup 4P_2, k-3)] \\
= \; & m(PPC_{n-1} \cup C_6, k) + m(PPC_{n-2} \cup 2P_5, k-1) + p_1m(PPC_{n-3} \cup 2P_5 \cup P_3, k-2) \\
& +p_2m(PPC_{n-3} \cup 2P_5 \cup P_4, k-2) + p_3m(PPC_{n-3} \cup 2P_5 \cup 2P_2, k-2) \\
& +p_1^2[p_1m(PPC^{1\prime}_{n-4} \cup P_5 \cup 2P_3, k-3) + p_2m(PPC^{2\prime}_{n-4} \cup P_5 \cup 2P_3, k-3) \\
& +p_3m(PPC^{3\prime}_{n-4} \cup P_5 \cup 2P_3, k-3)] \\
& +2p_1p_2[P_1m(PPC^{1\prime}_{n-4} \cup P_5 \cup P_3 \cup P_4, k-3) + p_2m(PPC^{2\prime}_{n-4} \cup P_5 \cup P_3 \cup P_4, k-3) \\
& +p_3m(PPC^{3\prime}_{n-4} \cup P_5 \cup P_3 \cup P_4, k-3)] \\
& +2p_1p_3[P_1m(PPC^{1\prime}_{n-4} \cup P_5 \cup P_3 \cup 2P_2, k-3) + p_2m(PPC^{2\prime}_{n-4} \cup P_5 \cup P_3 \cup 2P_2, k-3) \\
& +p_3m(PPC^{3\prime}_{n-4} \cup P_5 \cup P_3 \cup 2P_2, k-3)] \\
& +p_2^2[p_1m(PPC^{1\prime}_{n-4} \cup P_5 \cup 2P_4, k-3) + p_2m(PPC^{2\prime}_{n-4} \cup P_5 \cup 2P_4, k-3) \\
& +p_3m(PPC^{3\prime}_{n-4} \cup P_5 \cup 2P_4, k-3)] \\
& +2p_2p_3[p_1m(PPC^{1\prime}_{n-4} \cup P_5 \cup P_4 \cup 2P_2, k-3) + p_2m(PPC^{2\prime}_{n-4} \cup P_5 \cup P_4 \cup 2P_2, k-3) \\
& +p_3m(PPC^{3\prime}_{n-4} \cup P_5 \cup P_4 \cup 2P_2, k-3)] \\
& +p_3^2[p_1m(PPC^{1\prime}_{n-4} \cup P_5 \cup 4P_2, k-3) + p_2m(PPC^{2\prime}_{n-4} \cup P_5 \cup 4P_2, k-3) \\
& +p_3m(PPC^{3\prime}_{n-4} \cup P_5 \cup 4P_2, k-3)] \\
= \; & \cdots \\
= \; & m(PPC_{n-1} \cup C_6, k) \\
& + \sum_{t=0}^{n-2} \sum_{t_1+t_2+t_3=t} \tfrac{t!}{t_1!t_2!t_3!} p_1^{t_1} p_2^{t_2} p_3^{t_3} m(PPC_{n-2-t} \cup 2P_5 \cup t_1P_3 \cup t_2P_4 \cup 2t_3P_2, k-1-t)
\end{aligned}
$$

Since $\sum_{t_1+t_2+t_3=t} \tfrac{t!}{t_1!t_2!t_3!} p_1^{t_1} p_2^{t_2} p_3^{t_3} = (p_1+p_2+p_3)^t = 1$, and $m(M_{n-2-t} \cup 2P_5 \cup tP_3, k-1-t) \leq m(PPC_{n-2-t} \cup 2P_5 \cup t_1P_3 \cup t_2P_4 \cup 2t_3P_2, k-1-t) \leq m(O_{n-2-t} \cup 2P_5 \cup t_2P_4, k-1-t)$ by the inductive assumption and Lemma 2, we have

$$m(M_n, k) \leq m(PPC_n, k) \leq m(O_n, k)$$

for any $0 \leq k \leq 3n$. The induction is complete. □

Since $m(G, k) \geq m(H, k) \Leftrightarrow G \succ H$ for all k, and $G \succ H$ implies $ME(G) \geq ME(H)$, we have by Theorem 3

Theorem 4. *Let PPC_n be a random polyphenyl chain of length n. Then*

$$ME(M_n, k) \leq ME(PPC_n, k) \leq ME(O_n, k)$$

Specially, for the meta-chain M_n, the orth-chain O_n and the para-chain L_n, we have

Corollary 5. *(i)* $m(M_n, k) \leq m(L_n, k) \leq m(O_n, k)$ *for any* $0 \leq k \leq 3n$*; (ii)* $ME(M_n) \leq ME(L_n) \leq ME(O_n)$.

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