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The Number of Maximal Matchings in Polyphenylene Chains

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ABSTRACT

A matching is maximal if no other matching contains it as a proper subset. Maximal matchings model phenomena across many disciplines, including applications within chemistry. In this paper, we study maximal matchings in an important class of chemical compounds: polyphenylenes. In particular, we determine the extremal polyphenylene chains in regards to the number of maximal matchings. We also determine recurrences and generating functions for the sequences enumerating maximal matchings in several specific types of polyphenylenes and use these results to analyze the asymptotic behavior.

1. INTRODUCTION

A *matching* in a graph is a set of edges with no vertex in common. A matching is *maximum* in a graph if there is no matching with more edges. Matchings serve as mathematical models across many disciplines, with applications to engineering, network science, the social sciences, and natural sciences. One important application is specific to chemistry, where it was observed that the stability of benzenoid compounds is related to the number of perfect matchings, also known as *Kekulé structures*, in the corresponding graphs. The edges in a *perfect* matching are collectively incident to all the vertices in a graph, so these

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matchings are as large as possible. Perfect matchings are also maximum matchings, but the converse is not always true. There has been considerable work done on the enumeration and structure of perfect and maximum matchings [1,2].

A matching is *maximal* in a graph if no other matching contains it as a proper subset. Every maximum matching is maximal, but the converse is generally not true. A maximal matching is also an independent edge dominating set, that is, a set of independent edges that are collectively incident to all edges in a graph. See [3] for a survey on independent domination in graphs.

Within chemistry, maximal matchings serve as models to the adsorption of dimers on a substrate and the block-allocation of a sequential resource. They also appear in the polymerization of organic molecules [4]. Recently, there have been some enumerative results on the block allocation of a sequential resource [5] and maximal matchings in linear polymers [6,7]. The structure of maximal matchings has been studied for benzenoids [8], fullerenes [9,10], nanocones, and nanotubes [11,12].

A *phenylene* is a divalent radical derived from benzene by removing two hydrogen atoms. A polymer built from repeating phenylene units is called a *polyphenylene*. Polyphenylenes have attracted attention in the last few decades due to their good thermal and chemical resistance. They serve as a precursor for plastics used in engineering and medical applications as well as commercial products. Matchings in polyphenylenes have been studied [13,14] but nothing appears to be known about maximal matchings.

In this paper we add to the growing research on maximal matchings in chemical graphs by presenting some enumerative and extremal results on the number of maximal matchings in polyphenylene chains. Our main results are characterizations of the extremal polyphenylene chains in regards to the number of maximal matchings. Additionally, we obtain bivariate generating functions for the number of maximal matchings in three classes of uniform polyphenylene chains. These generating functions are then used to compute the asymptotics of the number of maximal matchings as well as the expected size of a maximal matching in these chains.

2. PRELIMINARIES

Throughout this paper, our terminology and notations are mostly taken from [2,15]. All graphs considered will be finite and simple with vertex set $V(G)$ and edge set $E(G)$. For a subset of the vertices S of $V(G)$, we use $G - S$ to denote the subgraph of G obtained by deleting the vertices of S and all edges incident to them. We will use $G - v$ or $G - \{v\}$ if S consists of a single vertex v. For a subset of the edges H of $E(G)$, we make use of the notation $G\backslash X$, or $G\backslash e$ if $X = \{e\}$, to denote the subgraph of G obtained by deleting the edges in X as well as all incident vertices to these edges.

A *matching* M in G is a set of edges with no vertex in common. The number of edges in M is called its *size*. A *maximum matching* is a matching of largest size. Let $\nu(G)$ denote the size of a maximum matching in a graph G, which is called the *matching number*. We call M a *maximal matching* if it is not a subset of a larger size matching in G. Let $\Psi(G)$ denote the number of maximal matchings of G.

A *cactus graph* (or cactus for short) is a connected graph in which no edge is contained in more than one cycle. So each block of a cactus is either an edge or a cycle. If all blocks of a cactus are cycles of the same length m, then the cactus is m*-uniform*.

A *hexagonal cactus* is a 6-uniform cactus. A vertex shared by two or more hexagons is called a cut vertex. A *chain hexagonal cactus* is a hexagonal cactus where each hexagon has at most two cut vertices and each cut vertex is shared by at most two hexagons. The number of hexagons in a chain hexagonal cactus is called the *length*. See Figure 1 for an example of a chain hexagonal cactus.

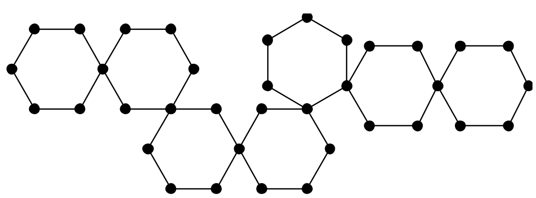

Figure 1. A chain hexagonal cactus of length 7.

A *polyphenylene chain* is a graph obtained from a hexagonal cactus by expanding each of its cut-vertices to an edge. Similarly, the *length* of a polyphenylene chain is the number of hexagons in the graph. See Figure 2 for the polyphenylene chain corresponding to the chain hexagonal cactus in Figure 1.

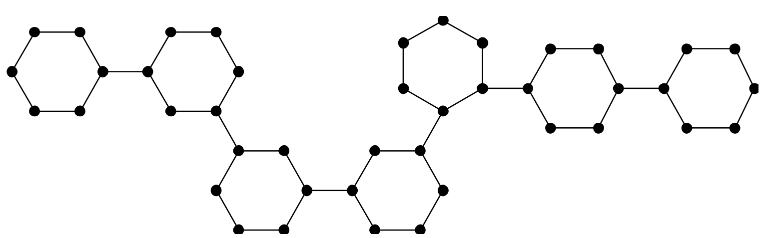

Figure 2. A polyphenylene chain of length 7.

Every polyphenylene chain contains exactly two hexagons with only one cut vertex. Those hexagons are called *terminal* and all other hexagons are called *internal*. Using terminology borrowed from benzenoid hydrocarbons, an internal hexagon is called a *para-hexagon*, a *meta-hexagon*, or an *ortho-hexagon* if its cut vertices are distance 3, 2, or 1, respectively. The unique chain of length n made up entirely of para-hexagons is called a *para-chain* denoted P_n. *Meta-chains* and *ortho-chains* are defined analogously and denoted by M_n and O_n, respectively, see Figures 3, 4, and 5.

3. STATEMENT OF RESULTS

In this section, we present bivariate generating functions for the number of maximal matchings of size k in the polyphenylene chains P_n, M_n, and O_n. To this end, we start by finding recursions for the number of such maximal matchings with the aid of several auxiliary graphs. A proof of Lemma 3.1 part (i) is presented in section 4 and the rest of the cases, including Lemmas 3.2 and 3.3, follow similarly. Initial conditions are determined by direct counting.

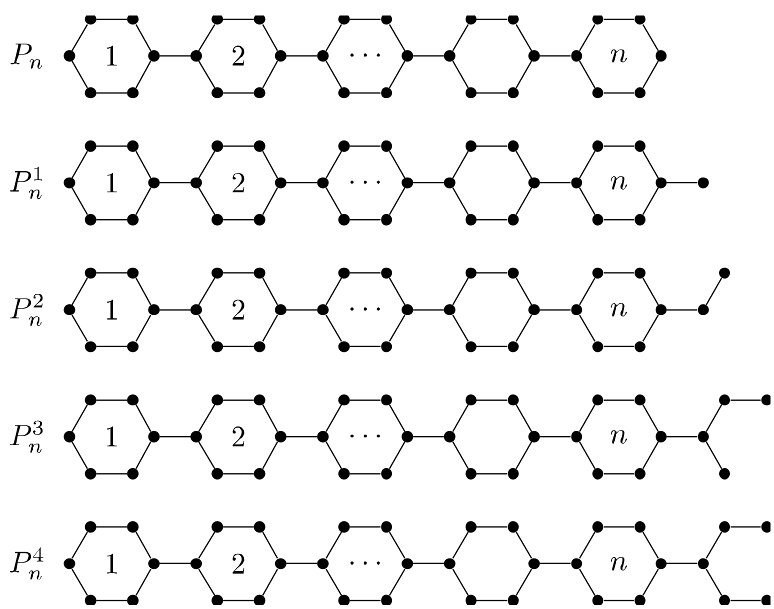

Figure 3. Auxiliary graphs for P_n.

Lemma 3.1. Let $p_{n,k}$ be the number of maximal matchings of size k in P_n and $p_{n,k}^i$ be the number of maximal matchings of size k in the auxiliary graph P_n^i in Figure 3. Then

1. $p_{n,k} = 2p^3_{n-1,k-1} + p^1_{n-1,k-2}$,
2. $p^1_{n,k} = p^4_{n-1,k-1} + 2p^3_{n-1,k-1}$,
3. $p^2_{n,k} = p_{n,k-1} + p^4_{n-1,k-1}$,
4. $p^3_{n,k} = p^2_{n,k-1} + p_{n,k-1}$,
5. $p^4_{n,k} = p^1_{n,k-2} + 2p_{n,k-2}$.

with $p_{0,0} = p^1_{0,0} = p^2_{0,1} = p^3_{0,2} = 1$, $p^3_{0,1} = 3$, $p^4_{0,1} = 4, p^4_{0,2} = 2$, and all other initial conditions equal to zero.

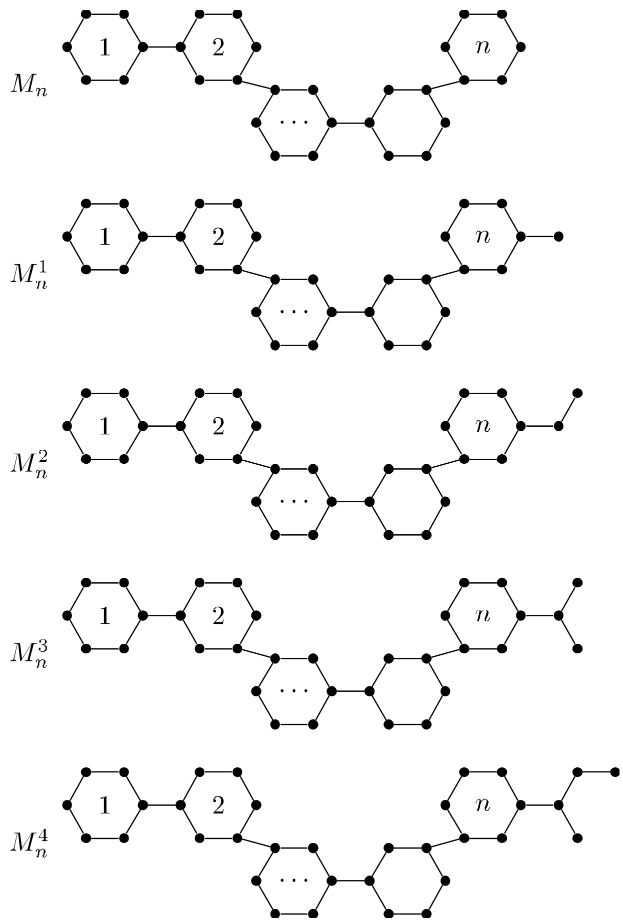

Figure 4. Auxiliary graphs for M_n.

Lemma 3.2. Let $m_{n,k}$ be the number of maximal matchings of size k in M_n and m_n^i be the number of maximal matchings of size k in the auxiliary graph M_n^i in Figure 4. Then

1. $m_{n,k} = 2m_{n-1,k-1}^4 + m_{n-1,k-2}^1$,
2. $m_n^1 = m_{n-1,k-1}^4 + m_{n-1,k-2}^3 + 2m_{n-1,k-2}^2 + m_{n-1,k-2}^1$,
3. $m_n^2 = m_{n,k-1} + m_{n-1,k-2}^3 + m_{n-1,k-2}^2$,
4. $m_n^3 = 2m_{n,k-1} + m_{n-1,k-2}^3 + m_{n-1,k-2}^2$,
5. $m_n^4 = m_{n,k-1}^2 + m_{n,k-1}$.

with $m_{0,0} = m_{0,0}^1 = m_{0,1}^2 = m_{0,2}^4 = 1$, $m_{0,1}^3 = 2$, $m_{0,1}^4 = 3$, and all other initial conditions equal to zero.

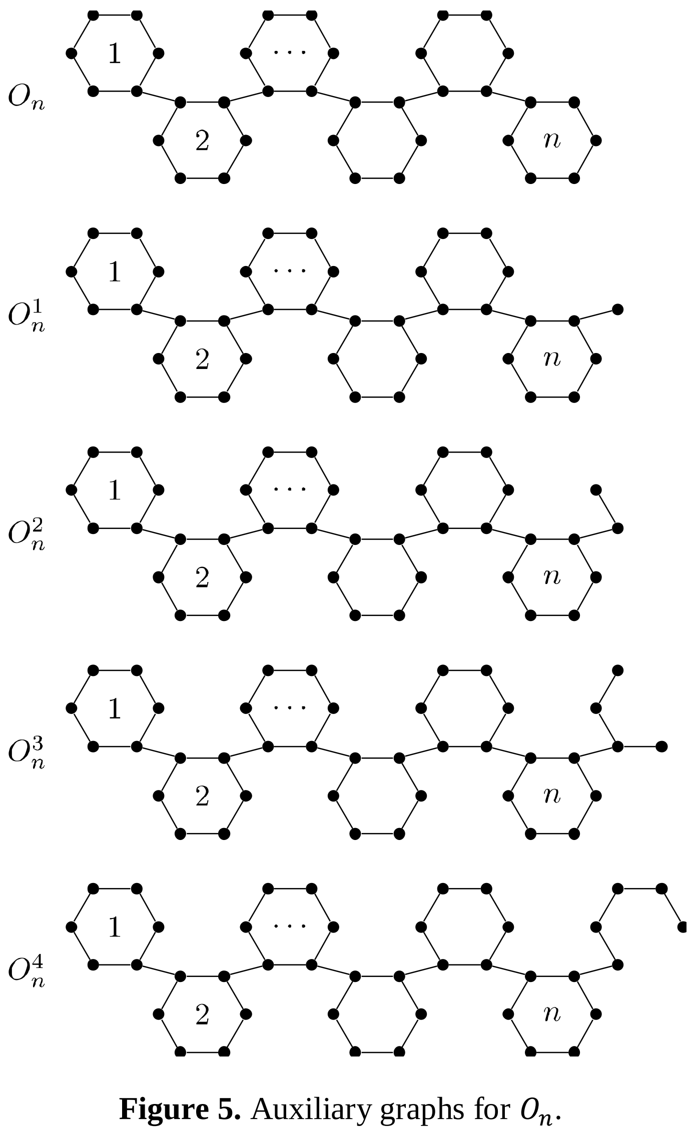

Figure 5. Auxiliary graphs for O_n.

Lemma 3.3. Let $o_{n,k}$ be the number of maximal matchings of size k in O_n and $o_{n,k}^i$ be the number of maximal matchings of size k in the auxiliary graph O_n^i in Figure 5. Then

1. $o_{n,k} = 2o_{n-1,k-1}^3 + o_{n-1,k-2}^1$,
2. $o_{n,k}^1 = o_{n-1,k-1}^4 + o_{n-1,k-2}^2 + o_{n-1,k-2}^1 + o_{n-1,k-2} + o_{n-1,k-3}$,
3. $o_{n,k}^2 = o_{n,k-1} + o_{n-1,k-1}^4$,
4. $o_{n,k}^3 = o_{n,k-1}^2 + o_{n,k-1}$,
5. $o_{n,k}^4 = o_{n,k-1}^2 + o_{n,k-2}^1 + o_{n,k-2}$.

with $o_{0,0} = o_{0,0}^1 = o_{0,1}^2 = o_{0,2}^3 = 1$, $o_{0,1}^3 = 3$, $o_{0,1}^4 = 4$, $o_{0,2}^4 = 3$, and all other initial conditions equal to zero.

We can now use the five recursions presented in Lemma 3.1 to solve a system of equations involving five unknown, bivariate generating functions for the sequences $p_{n,k}$ and $p_{n,k}^i$. Similarly, we can use Lemmas 3.2 and 3.3 to solve for the bivariate generating functions for the sequences $m_{n,k}$ and $o_{n,k}$. We omit the computation details and present the results below.

Proposition 3.4. Let $P(x,y)$, $M(x,y)$, and $O(x,y)$ be the bivariate generating functions for the sequences $p_{n,k}$, $m_{n,k}$, and $o_{n,k}$, respectively. Then

1. $P(x,y) = \frac{xy^3-xy^2-1}{4x^3y^7-2x^2y^6+8x^2y^5+2x^2y^4+3xy^3+2xy^2-1}$,
2. $M(x,y) = \frac{2xy^2-1}{x^3y^7+3x^3y^6-7x^2y^4-2x^3y^5+4x^2y^5+x^2y^3+7xy^2-1}$,
3. $O(x,y) = \frac{-x^2y^5+xy^3+xy^2-1}{2x^3y^8-2x^3y^7+3x^2y^5+(x^3-2x^2)y^6-4x^2y^4+3xy^3+4xy^2-1}$.

Let p_n, m_n, and o_n be the sequences for the number of maximal matchings in the polyphenylene chains P_n, M_n, and O_n, respectively. Then substituting $y = 1$ into Proposition 3.4 we can obtain the ordinary generating functions for these sequences.

Corollary 3.5. Let $P(x)$, $M(x)$, and $O(x)$ be the ordinary generating functions for the sequences p_n, m_n, and o_n, respectively. Then

1. $P(x) = \frac{-1}{4x^3+8x^2+5x-1}$,
2. $M(x) = \frac{2x-1}{2x^3-2x^2+7x-1}$,
3. $O(x) = \frac{-x^2+2x-1}{x^3-3x^2+7x-1}$.

Since the generating functions for $P(x)$, $M(x)$, and $O(x)$ are all rational functions, we may conclude that p_n, m_n, and o_n each satisfy a third order linear recurrence with constant coefficients. The initial conditions are found by direct computation.

Corollary 3.6.

1. $p_n = 5p_{n-1} + 8p_{n-2} + 4p_{n-3}$

with initial conditions $p_0 = 1$, $p_1 = 5$, $p_2 = 33$

2. $m_n = 7m_{n-1} - 2m_{n-2} + 2m_{n-3}$

with initial conditions $m_0 = 1$, $m_1 = 5$, $m_2 = 33$,

3. $o_n = 7o_{n-1} - 3o_{n-2} + o_{n-3}$

with initial conditions $o_0 = 1$, $o_1 = 5$, $o_2 = 33$.

Having found the generating functions, a variant of Darboux's theorem [16] can be applied to deduce the asymptotic behavior of the sequences p_n, m_n, and o_n. The theorem is stated below as Theorem 3.7.

Theorem 3.7. (Darboux). Let $f(x) = \sum_0^\infty a_n x^n$ denote the ordinary generating function of a sequence a_n. If $f(x)$ can be written as

$$f(x) = \left(1 - \frac{x}{w}\right)^\alpha g(x),$$

such that w is the smallest modulus singularity of f and g is analytic at w, then

$$a_n \sim \frac{g(w)}{\Gamma(-\alpha)} w^{-n} n^{-\alpha-1},$$

where $\Gamma(x)$ denotes the gamma function.

Since the ordinary generating functions $P(x)$, $M(x)$, and $O(x)$ all have a real root (which is their smallest modulus singularity), Theorem 3.7 may be applied to them to determine the asymptotic behavior of each sequence. Also, since each of these roots has a multiplicity of 1, all of the sequences will have asymptotic behavior that follows an exponential function. While the generating functions provide enough information to find an explicit formula for any of these sequences, the resulting equations would be too complicated to be of much practical use, so below we give approximations. We omit the computations and present only the final results.

Corollary 3.8.

1. $p_n \sim 0.813618 \cdot 6.357356^n$,
2. $m_n \sim 0.726021 \cdot 6.747523^n$,
3. $o_n \sim 0.766527 \cdot 6.566316^n$.

Comparing the asymptotics of each chain, it seems that the meta-chains have the most possible maximal matchings, while the para-chains have the fewest of all possible polyphenylene chains. We will later prove that this is, in fact, the case.

Again using Theorem 3.7 we can compute the expected size of a maximal matching in the chains P_n, M_n, and O_n. Let $\pi(G)$ denote the expected size of a maximal matching in a graph G. Let G_n be a polyphenylene chain of length n, let $g_{n,k}$ be the number of maximal matchings of size k in G_n, and let $G(x,y) = \sum_{k=0}^{\nu(G)} g_{n,k}\, x^n y^k$ be the bivariate generating function for $g_{n,k}$. Then the expected size of a maximal matching in G_n is

$$\pi(G_n) = \frac{[x^n]\frac{\partial G(x,y)}{\partial y}\big|_{y=1}}{[x^n]G(x,y)\big|_{y=1}},$$

where $[x^n]F(x)$ denotes the coefficient of x^n in the expansion of $F(x)$. We omit the computational details and present the result below.

1. $\pi(P_n) \approx 2.477132700n$,
2. $\pi(M_n) \approx 2.07807029n$,
3. $\pi(O_n) \approx 2.47013906n$

The efficiency $\varepsilon(G)$ of a random maximal matching on a graph G is the ratio of the expected size of a maximal matching and its matching number, that is, $\varepsilon(G) = \frac{\pi(G)}{\nu(G)}$. Since each of P_n, M_n, and O_n have perfect matchings of size $3n$, we immediately get that

$$\begin{aligned} \varepsilon(P_n) &= 0.8257, \\ \varepsilon(M_n) &= 0.6927, \\ \varepsilon(O_n) &= 0.8234. \end{aligned}$$

These results show para and ortho chains have similar expected sizes of maximal matchings and efficiency, while meta chains are lower. One explanation for this concerns the edges between the hexagons. In a meta chain, if both edges adjacent to a hexagon are in a maximal matching, then only one edge from the hexagon is saturated by the matching. While in para and ortho chains, if both edges adjacent to the hexagon are in a maximal matching, then up to two edges from the hexagon can be in the matching.

We conclude the section with our main result concerning the extremal polyphenylene chains in regards to the number of maximal matchings, which is proved in the following section.

Theorem 3.9. Let G_n be a polyphenylene chain of length n. Then

$$\Psi(P_n) \leq \Psi(G_n) \leq \Psi(M_n).$$

4. PROOFS

Let G_m be an arbitrary polyphenylene chain of length m. Observe that we can always draw G_m as in Figure 6, where h_m is a terminal hexagon and the hexagon adjacent to the left of h_{m-1} may attach at any of the vertices a, b, c, e, or f. Let us assume the hexagons of G_m are labeled h_1, h_2, ..., h_m according to their ordering in Figure 6 (where h_1 is the other terminal hexagon).

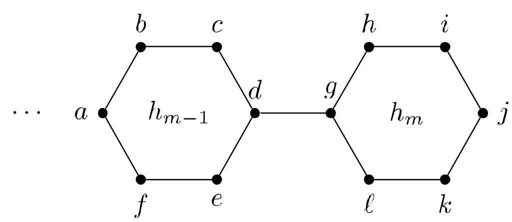

Figure 6. A terminal hexagon h_m and its adjacent hexagon h_{m-1} in the polyphenylene chain G_m.

For any $1 \leq p \leq q \leq m$, let H_p represent the subgraph of G_m induced by the vertices of the hexagons h_1, h_2, ... h_p, and let $H_{p,q}$ denote the subgraph of G_m induced by the vertices of the hexagons h_p, h_{p+1}, ... h_q.

Proof (of Lemma 3.1). Here we prove part (i) since the remaining parts follow similarly. Suppose P_n is drawn in Figure 7 where h_n is a terminal hexagon. Any size k maximal matching of P_n must contain exactly one of the edges ij or jr, or the maximal matching must contain both of the edges hi and ℓr. If a maximal matching contains the edge ij, then the remaining edges form a maximal matching of size $k-1$ in the graph P_{n-1}^3. By symmetry, the same holds for any maximal matching containing the edge jr. If the maximal matching contains the edges hi and ℓr, then the remaining edges form a maximal matching of size $k-2$ of the graph P_{n-1}^1. Thus, the recursion $p_{n,k} = 2p_{n-1,k-1}^3 + p_{n-1,k-2}^1$ holds. ∎

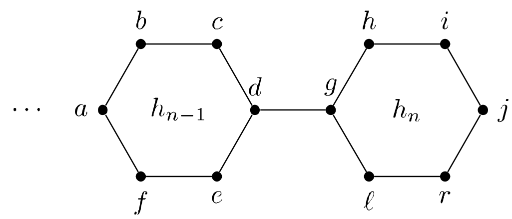

Figure 7. The polyphenylene chain P_n.

In order to provide quicker rationale for decisions later, we consider this lemma involving the arrangement of edges in a matching surrounding any given vertex.

Lemma 4.1. For any vertex v and maximal matching M of G, one of the following must hold:

1. M contains an edge incident to v, or
2. for each vertex $a \in N(v)$, M contains exactly one edge incident to a.

Proof. Suppose that M does not contain an edge incident to v and there exists $a \in N(v)$ such that no edge in M is incident to a. Then we could add the edge va to M, which is a contradiction to the fact that M is maximal. ∎

In order to compare the total number of matchings between the possible terminating hexagon configurations, we will first establish a few lemmas that will enable a comparison between the (total) number of matchings in different subgraphs.

Lemma 4.2. If H is a subgraph of the graph G, then $\Psi(H) \leq \Psi(G)$.

Proof. This directly follows from the fact that every maximal matching in H can be extended to at least one maximal matching in G. ∎

Lemma 4.3.

i. $\Psi(H_{m-1}) \geq \Psi(H_{m-1} - \{c, d\}) + \Psi(H_{m-1} - \{d, e\})$
ii. $\Psi(H_{m-1}) \leq \Psi(H_{m-1} - \{c, d\}) + \Psi(H_{m-1} - \{d, e\}) + \Psi(H_{m-1} - d)$

Proof. Let us consider the subgraph H_{m-1}. The preceding hexagon h_{m-2} (in cases such that $m \geq 3$) may be attached at any of the vertices a, b, c, e, or f. Due to the symmetry of vertices b and c to vertices f and e, respectively, we may assume without loss of generality that h_{m-2} attaches to a, f, or e. Now, we consider the vertex d. By applying Lemma 4.1, we conclude that any maximal matching must contain exactly one of the edges cd and de, or it must contain two edges (excluding cd and de), one that ends at c and one that ends at e. These cases are considered below:

Case 1. The edge cd is contained in the matching:

Here, the total number of maximal matchings is equal to those of the graph after the vertices c and d are removed from the graph, so there are $\Psi(H_{m-1} - \{c, d\})$ such matchings.

Case 2. The edge de is contained in the matching:

In this case, the total number of maximal matchings is equal to those of the graph after the vertices d and e are removed from the graph, so there are $\Psi(H_{m-1} - \{d, e\})$ such matchings.

Case 3. Other edges, one that ends at c and one that ends at e are part of the matching:

The edges used in this last case are bc and either fe or the edge connecting h_{m-2} to h_{m-1}, in the case that h_{m-1} is an ortho-hexagon. In either case, let H_{m-1}^{-} denote the subgraph obtained by removing said pair of edges are in the matching. Note that, since the chosen edges include c and e as endpoints, $c, e \notin H_{m-1}^{-}$. With the removal of these vertices, the edges cd and de are also removed, implying that $H_{m-1}^{-} \subset H_{m-1} - d$.

Thus,

$$\Psi(H_{m-1}) = \Psi(H_{m-1} - \{c, d\}) + \Psi(H_{m-1} - \{d, e\}) + \Psi(H_{m-1}^{-}).$$

We draw two conclusions from this equation. First, since any graph, even an empty one, has a positive number of maximal matchings, $\Psi(H_{m-1}^{-}) > 0$, and therefore

$$\Psi(H_{m-1}) \geq \Psi(H_{m-1} - \{c, d\}) + \Psi(H_{m-1} - \{d, e\}),$$

which proves part (i).

Second, since we know the graph $\Psi(H_{m-1}^{-})$ to be a subgraph of $H_{m-1} - d$, then $\Psi(H_{m-1}^{-}) \leq \Psi(H_{m-1} - d)$. As a result, we get that

$$\Psi(H_{n-2}) \leq \Psi(H_{n-2} - \{c, d\}) + \Psi(H_{n-2} - \{d, e\}) + \Psi(H_{n-2} - d),$$

which is part (ii). ■

Proof (of Theorem 3.10). Consider a polyphenylene chain C of length $n-1$. Suppose that C is drawn as in Figure 6 with the same labeled vertices (where $m = n-1$). We will then consider the possible cases of extending C by adding an nth hexagon h_n.

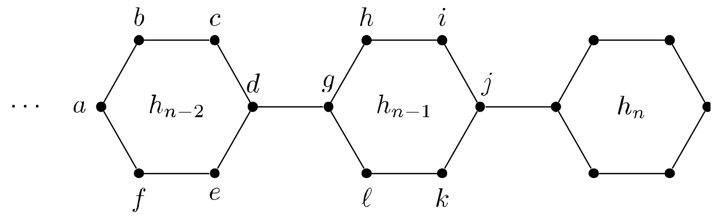

Figure 8. The polyphenylene chain CP.

Case 1. Let h_{n-1} be a para-hexagon, so that h_n attaches at the vertex j, as shown above in Figure [para_extremal_case]. We will denote the resulting graph as CP. To compute $\Psi(CP)$, we will consider the vertex g and apply Lemma 4.1 to determine the various cases involved. According to the lemma, there must be exactly one of the edges dg, gh, and gl in any maximal matching; otherwise the matching may not contain any of those three edges and must instead contain the edges hi, lk, and either cd or de. These cases will each be considered in turn below.

Case 1a. The edge dg is in the matching.

In this case, the remaining edges of the matching will form maximal matchings of $H_{n-2} - d$ and $H_{n-1,n} - g$. By direct counting of the maximal matchings of $H_{n-1,n} - g$, we find that $\Psi(H_{n-1,n} - g) = 17$. Thus, this case will contribute $17 \cdot \Psi(H_{n-2} - d)$ to the total number of maximal matchings.

Case 1b. Either gh or gl are in the matching.

In the case that either gh or gl is selected, the remaining edges form maximal matchings of H_{n-2} and either $H_{n-1,n} - \{g,h\}$ or $H_{n-1,n} - \{g,l\}$, respectively. By direct counting and symmetry, $\Psi(H_{n-1,n} - \{g,h\}) = \Psi(H_{n-1,n} - \{g,l\}) = 13$. Thus, another $26 \cdot \Psi(H_{n-2})$ is contributed to $\Psi(CP)$.

Case 1c. The edges hi, lk, and exactly one of cd and de are in the matching.

In this final case, if either cd or de is selected, the remaining edges form maximal matchings of $H_{n-2} - \{c,d\}$ or $H_{n-2} - \{d,e\}$, respectively, as well as $H_{n-1,n} - \{g,h,i,k,l\}$. By counting the number of matchings included in this last subgraph, we find $\Psi(H_{n-1,n} - \{g,h,i,k,l\}) = 7$. This contributes a final $7(\Psi(H_{n-2} - \{c,d\}) + \Psi(H_{n-2} - \{d,e\}))$ to the total maximal matchings.

We may determine $\Psi(CP)$ by summing all of the matchings contributed by the three cases listed above. Thus, we conclude that

$$\Psi(CP) = 26 \cdot \Psi(H_{n-2}) + 17 \cdot \Psi(H_{n-2} - d) + 7(\Psi(H_{n-2} - \{c,d\}) + \Psi(H_{n-2} - \{d,e\}))$$

and let us denote this as equation (1).

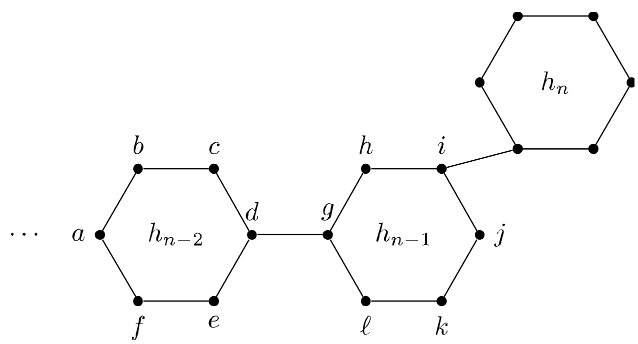

Figure 9. The polyphenylene chain, CM.

Case 2. Let the hexagon h_{n-1} be a meta-hexagon, so that h_n attaches at either vertex i or k. Without loss of generality assume that h_n attaches to i, as shown in Figure 9. We will denote the resulting graph as CM. To compute $\Psi(CM)$, we will again consider vertex g and apply Lemma 4.1, yielding the following cases:

Case 2a. The edge dg is in the matching.

In this case, the remaining edges of the matching will form maximal matchings of $H_{n-2} - d$ and $H_{n-1,n} - g$. By direct counting of the maximal matchings of $H_{n-1,n} - g$, we find that $\Psi(H_{n-1,n} - g) = 21$. Thus, this case will contribute $21 \cdot \Psi(H_{n-2} - d)$ to the total number of maximal matchings

Case 2b. Either gh or gl are included in the matching.

In the case that either gh or gl is selected, the remaining edges form maximal matchings of H_{n-2} and either $H_{n-1,n} - \{g,h\}$ or $H_{n-1,n} - \{g,l\}$, respectively. These subgraphs are not symmetric and counting them individually we find that $\Psi(H_{n-1,n} - \{g,h\}) = 15$ and $\Psi(H_{n-1,n} - \{g,l\}) = 13$. Thus, another $28 \cdot \Psi(H_{n-2})$ is contributed to $\Psi(CM)$.

Case 2c. The edges hi, lk, and exactly one of cd and de are in the matching.

In this final case, we observe that if either cd or de is selected, the remaining edges form maximal matchings of $H_{n-2} - \{c,d\}$ or $H_{n-2} - \{d,e\}$, respectively, as well as $H_{n-1,n} - \{g,h,i,k,l\}$. By counting the number of matchings included in this last subgraph, we find $\Psi(H_{n-1,n} - \{g,h,i,k,l\}) = 5$. This contributes a final $5(\Psi(H_{n-2} - \{c,d\}) + \Psi(H_{n-2} - \{d,e\}))$ to the total maximal matchings.

From the above cases, we may determine $\Psi(CM)$ by summing all of the matchings contributed by each case. Thus, we conclude

$$\Psi(CM) = 28 \cdot \Psi(H_{n-2}) + 21 \cdot \Psi(H_{n-2} - d) + 5(\Psi(H_{n-2} - \{c,d\}) + \Psi(H_{n-2} - \{d,e\}))$$

and let us denote this as equation (2).

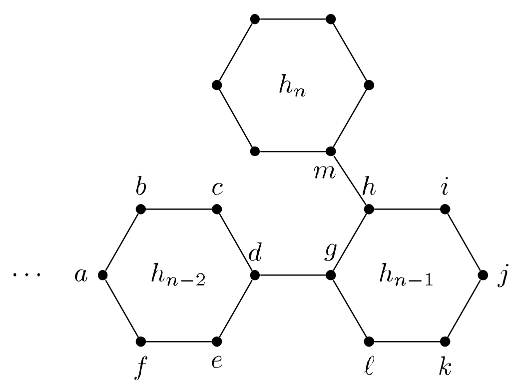

Figure 10. The polyphenylene chain, CO.

Case 3. Let h_{n-1} be an ortho-hexagon, so that h_n attaches to vertex h or ℓ. Without loss of generality assume that h_n attaches to h, as shown above in Figure 10. We will denote the resulting graph as CO. To compute $\Psi(CO)$, we will consider the vertex g and apply Lemma 4.1 as before. The resulting cases are as follows:

Case 3a. The edge dg is in the matching.

In this case, the remaining edges of the matching will form maximal matchings of $H_{n-2} - d$ and $H_{n-1,n} - g$. By direct counting of the maximal matchings of $H_{n-1,n} - g$, we find that $\Psi(H_{n-1,n} - g) = 20$. Thus, this case will contribute $20 \cdot \Psi(H_{n-2} - d)$ to the total number of maximal matchings

Case 3b. Either gh or gl are in the matching.

In the case that either gh or gl is selected, the remaining edges form maximal matchings of H_{n-2} and either $H_{n-1,n} - \{g, h\}$ or $H_{n-1,n} - \{g, l\}$, respectively. By direct counting we find that $\Psi(H_{n-1,n} - \{g, h\}) = 10$ and $\Psi(H_{n-1,n} - \{g, l\}) = 15$. Hence, another $25 \cdot \Psi(H_{n-2})$ is added to $\Psi(CM)$.

Case 3c. The edges kl, either hi or hm, and either cd or de are included in the matching.

If either cd or de is in the matching, the remaining edges form a maximal matching of $H_{n-2} - \{c, d\}$ or $H_{n-2} - \{d, e\}$, respectively, as well as either $H_{n-1,n} - \{g, h, i, k, l\}$ or $H_{n-1,n} - \{g, h, k, l, m\}$. By counting the number of matchings, we find $\Psi(H_{n-1,n} - \{g, h, i, k, l\}) = 5$ and $\Psi(H_{n-1,n} - \{g, h, k, l, m\}) = 3$. This contributes a final $8(\Psi(H_{n-2} - \{c, d\}) + \Psi(H_{n-2} - \{d, e\}))$ to the total number of maximal matchings.

From these cases, we may determine $\Psi(CO)$ by summing all of the matchings contributed by the three cases above. Thus, we conclude that

$$\Psi(CO) = 25 \cdot \Psi(H_{n-2}) + 20 \cdot \Psi(H_{n-2} - d) + 8\big(\Psi(H_{n-2} - c, d) + \Psi(H_{n-2} - d, e)\big)\#$$

and let us denote this as equation (3).

We now begin to compare these equations for the number of maximal matchings in each of the three configurations. To show that $\Psi(CM) > \Psi(CO)$, by applying Lemma 4.3 part (i) to equation(2) and directly comparing terms, we get

$$\begin{aligned}\Psi(CM) &= 28\Psi(H_{n-2}) + 21\Psi(H_{n-2} - d) + 5(\Psi(H_{n-2} - \{c, d\}) + \Psi(H_{n-2} - \{d, e\}))\\ &\geq 25\Psi(H_{n-2}) + 21\Psi(H_{n-2} - d) + 8(\Psi(H_{n-2} - \{c, d\}) + \Psi(H_{n-2} - \{d, e\}))\\ &\geq 25\Psi(H_{n-2}) + 20\Psi(H_{n-2} - d) + 8(\Psi(H_{n-2} - \{c, d\}) + \Psi(H_{n-2} - \{d, e\}))\\ &= \Psi(CO).\end{aligned}$$

Similarly, to show that $\Psi(CO) > \Psi(CP)$ we apply Lemma 4.3 part (ii) to equation (3) to get

$$\begin{aligned}\Psi(CO) &= 25\Psi(H_{n-2}) + 20\Psi(H_{n-2} - d) + 8(\Psi(H_{n-2} - \{c, d\}) + \Psi(H_{n-2} - \{d, e\}))\\ &\geq 26\Psi(H_{n-2}) + 19\Psi(H_{n-2} - d) + 7(\Psi(H_{n-2} - \{c, d\}) + \Psi(H_{n-2} - \{d, e\}))\\ &\geq 26\Psi(H_{n-2}) + 17\Psi(H_{n-2} - d) + 7(\Psi(H_{n-2} - \{c, d\}) + \Psi(H_{n-2} - \{d, e\}))\\ &= \Psi(CP).\end{aligned}$$

Having shown that $\Psi(CM) \geq \Psi(CO) \geq \Psi(CP)$, the proof is complete. ■

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