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LABELLING AND COMPARISON OF ISOMERIC TREE-LIKE POLYPHENYL SYSTEMS

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Abstract

Tree-like polyphenyl systems form an important class of compounds in chemistry, in particular material science and polymers. The importance can be seen in LEDs, transmitters, and electronics. In recent years, many extremal results regarding such systems under specific constraints have been reported. More specifically are the sub-categories of such systems with extremal Wiener indices. In this article, we provide a labelling of the vertices on each hexagon (i.e., the corresponding benzene ring), which facilitates the illustration of a tree-like polyphenyl system with its corresponding tree structure. This approach helps to characterize the extremal tree-like polyphenyl systems with respect to the Wiener index and compare such systems in general within isometric molecules and between molecules of different underlying tree structures. The results can be used to order these systems, which will aid in predicting the physical properties of compounds. We also briefly examined tree-like polyphenyl systems that resulted from different tree structures.

1. Introduction

Polyphenyl compounds are synthetically or naturally derived compounds composed of multiple phenyl rings. These compounds can sometimes be hard to isolate and characterize due to the high variability and probability of impurities associated with their synthesis [20]. Therefore, the properties that have been reported are usually determined in large batches or are a mixture of the various formations. These compounds have been known to be useful in the area of material science and polymer chemistry, which include organic light emitting diodes, catalysts, and transmitters, along with some biological applications [15]. They have also been used in molecular models of graphene as well as discotic liquid crystals due to their higher solubilities, high thermal stability, and lowered melting points [9]. The integration of polyphenyl compounds to polymer backbones have been shown in various studies to increase the high glass transition temperature (T_g), lower the degree of molecular association, and even create a transparent film all the while conserving the properties of the original polymer [9]. It will be helpful to be able to predict properties of these compounds due to the associated applications, costly nature of synthesis, and purification techniques as well as the wide physical range of properties and conformations.

In this article, we will refer to the rings simply as “hexagons”. A polyphenyl system Z is “tree-like” if each vertex of Z lies on exactly one hexagonal plane and the graph obtained by contracting each hexagon into a vertex is a *tree* (that is, a connected graph with no cycle; Figure 1).

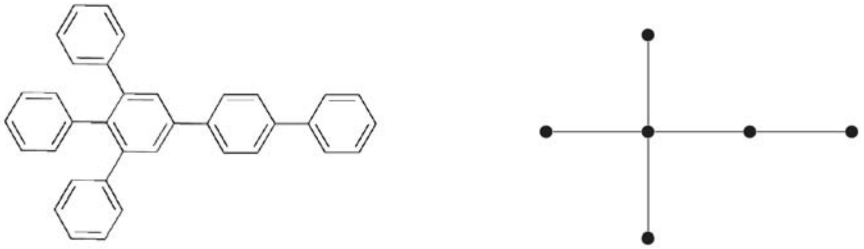

Figure 1. A tree-like polyphenyl system and the corresponding tree.

Two adjacent vertices in the tree structure correspond to the two hexagons joined by an edge. Each vertex (on a hexagon) is incident to no more than one of the edges joining hexagons and each vertex belongs to exactly one hexagon. For instance, Figure 2 shows an example of a structure that is not a tree-like polyphenyl systems. The structure has two vertices that are shared by more than one hexagon.

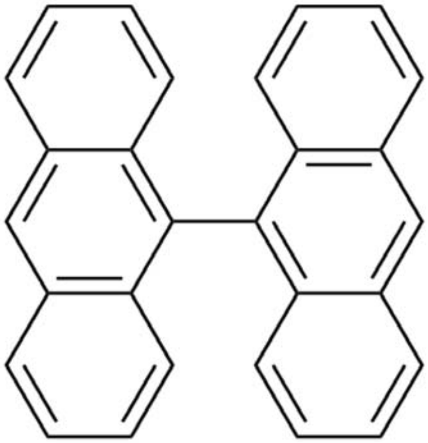

Figure 2. Example of a structure that is not a tree-like polyphenyl system.

Topological indices have been used as a convenient abstraction of chemical structures and have shown strong correlations with the chemical's physical properties. Throughout the years, numerous such indices are proposed, known as the chemical indices, for various categories of chemical structures. One of the most well-known such indices is due to and later named after Harry Wiener ([22]).

For a graph G with vertex set $V(G)$ and edge set $E(G)$, the Wiener index of G is defined as the sum of the lengths of the shortest paths between all pairs of vertices in the chemical graph representing the non-hydrogen atoms in the molecule or mathematically as

$$W(G) = \sum_{u, v \in V(G)} d(u, v),$$

where $d(u, v)$ denotes the distance between u and v (the number of edges on the shortest path connecting u and v) and the sum goes over all unordered pairs of vertices of G.

In the past decade, the maximum and minimum Wiener index of different categories of structures have been recently studied and the extremal structures have been characterized. See, for instance, [5, 7, 11, 12, 18, 19, 21, 24] for some (but certainly not all) of a variety of studies on the Wiener index and related concepts on trees. In recent years, similar studies have been conducted on some specific tree-like polyphenyl systems [2] and specific questions on such systems have been of interests [6, 23].

In this article, we present a simple labelling system of hexagonal vertices that enables concise tree representations of tree-like polyphenyl systems in Section 2. In Section 3, we provide the explicit characteristics of the extremal structures that minimize the Wiener index among tree-like polyphenyl systems with the same underlying tree structure. It is noted that our findings, in addition to identifying the extremal structures, also enables us to officially compare isomeric tree-like polyphenyl systems through the value of their Wiener indices. We further discuss the impact of different tree structures on the polyphenyl systems in Section 4, through the consideration of pairs of adjacent hexagons. A natural ordering (according to the value of the Wiener index) of simple systems follows as an immediate consequence and the results are compared with some of the predicted physical properties in Section 5, showing potential of the proposed approach in predicting physical-chemical properties. Lastly, in Section 6, we comment on the results and propose some future topics of study.

2. Labelling of Hexagonal Vertices

Evidently different tree-like polyphenyl systems may be reduced to the same tree. For instance, Figure 3 is a different tree-like polyphenyl system from that in Figure 1 but it still reduces to the same tree structure after contraction of hexagons.

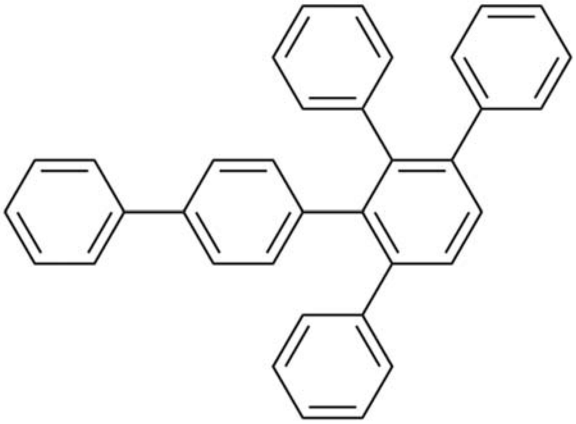

Figure 3. A different polyphenyl system.

For the purpose of distinguishing such systems with the same tree structure, we label the vertices on each hexagon with 1, 2, 4, 6, 5, 3 in the clockwise order as in Figure 4.

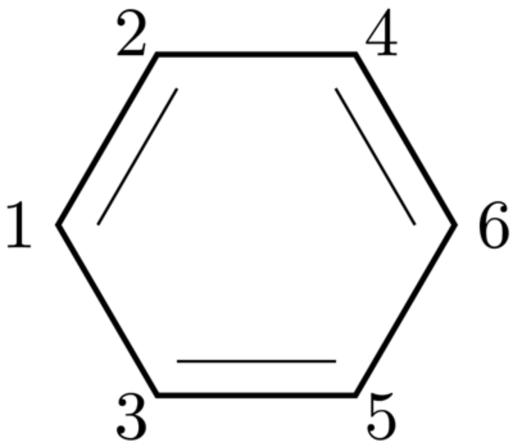

Figure 4. Labelling of an aromatic ring in a tree-like system.

Remark 1. This labelling of an aromatic ring, although seemingly unusual, emphasizes the importance of adjacent and opposite atoms of this aromatic ring in the tree-like system. The numbering is indeed coherent with the ordering of branching sizes when the Wiener index is minimized.

For an edge connecting two vertices from different hexagons in a tree-like system, we label the two end of this edge to denote where is the hexagon connected to this edge. For instance, the system in Figure 1 can now be represented as Figure 5.

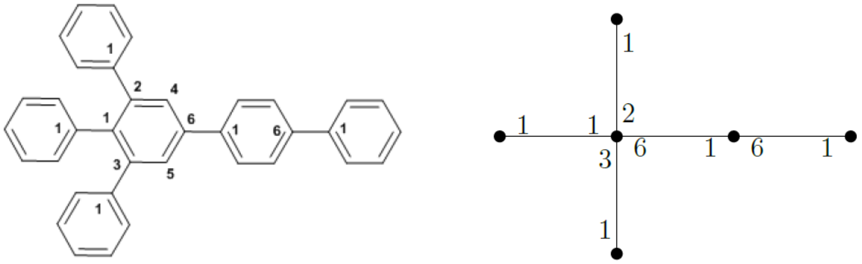

Figure 5. Labelling and tree representation with edge labels for Figure 1.

We omit an edge label if it does not affect the tree-like system. In particular, we do not label the leaf-ends of pendant edges. Figure 6 shows another example with such labellings. Note that this example denotes a different system that shares exactly the same tree structure.

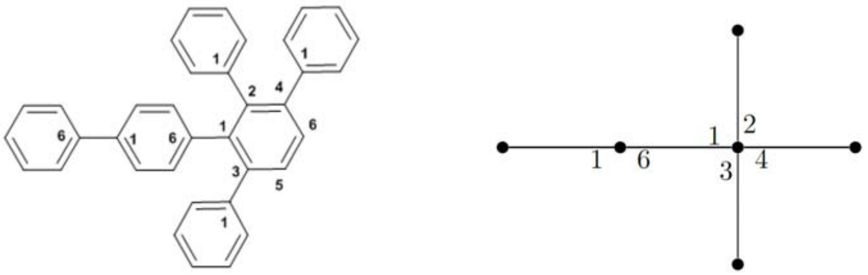

Figure 6. A different edge labelling pattern for Figure 3 with same tree-like structure.

3. Tree-like Polyphenyl System with a Given Tree Structure

Here we consider polyphenyl systems Z with a given underlying tree structure T. First recall that the Wiener index of a tree T can also be represented by

$$W(T) = \sum_{uv \in E(T)} n(u)n(v),$$

where $n(u)$ and $n(v)$ are the numbers of vertices in T closer to u and v, respectively. Following the same idea, we have

Proposition 3.1. *The number of times an edge* $uv \in E(T)$ *is used as part of a path in* Z *is*

$$(6n(u)) \cdot (6n(v)) = 36n(u)n(v).$$

The sum of these values for all edges in T *is*

$$36W(T).$$

Consequently

$$W(Z) = 36W(T) + C(Z),$$

where $C(Z)$, the contribution to $W(Z)$ from hexagonal edges, is the only variable that we need to consider (since $W(T)$ is a constant when T is given).

Let the components resulted from removing the edges of a hexagon in Z be denoted by $Z_1, \dots, Z_6$ (Figure 7) according to the labelling of the vertices on the aromatic ring, drawn here and throughout the rest of the article as a hexagon. Each component contains a polyphenyl system based around a central aromatic ring.

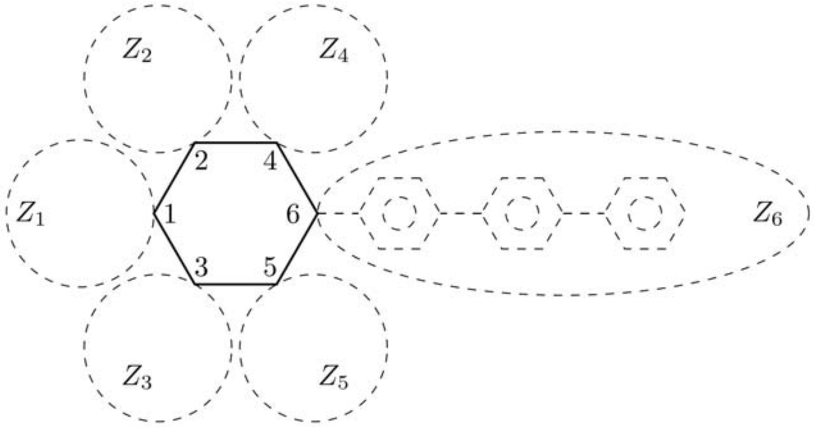

Figure 7. Z, represented by a hexagon and the resulted components.

Take, for instance, a vertex $v_2 \in Z_2$ and a vertex $v_6 \in Z_6$, the contribution of edges on this hexagon to $d(v_2, v_6)$ is 2. Hence the total contribution of this hexagon to distances between vertices in Z_2 and Z_6 is $2z_2z_6$, where $z_i = |V(Z_i)|$ for $1 \le i \le 6$. Taking all pairs of components into consideration, we have the contribution of this hexagon to $C(Z)$ as

$$(z_1z_2 + z_1z_3 + z_2z_4 + z_3z_5 + z_4z_6 + z_5z_6)$$

$$+ 2(z_1z_4 + z_1z_5 + z_2z_6 + z_3z_6 + z_2z_3 + z_4z_5)$$

$$+ 3(z_1z_6 + z_2z_5 + z_3z_4)$$

$$= (z_1 + z_2 + z_3 + z_4 + z_5 + z_6)^2 - (z_1^2 + z_2^2 + z_3^2 + z_4^2 + z_5^2 + z_6^2)$$

$$+ (z_1z_6 + z_2z_5 + z_3z_4) - (z_1z_2 + z_1z_3 + z_2z_4 + z_3z_5 + z_4z_6 + z_5z_6).$$

Note that, with given underlying tree structure and choice of the hexagon under consideration, both

$$(z_1 + z_2 + z_3 + z_4 + z_5 + z_6)^2 = |V(G)|^2,$$

and

$$(z_1^2 + z_2^2 + z_3^2 + z_4^2 + z_5^2 + z_6^2),$$

are constants. Hence we only need to focus our attention on

$$(z_1z_6 + z_2z_5 + z_3z_4) - (z_1z_2 + z_1z_3 + z_2z_4 + z_3z_5 + z_4z_6 + z_5z_6), \tag{1}$$

with given values of z_i.

We will show that, with given choices of Z_i's but exibility to rearrange them, (1) is minimized when the components is arranged in a way such that

$$z_1 \geq z_2 \geq z_3 \geq z_4 \geq z_5 \geq z_6, \tag{2}$$

i.e., the "largest" component is attached to the hexagon at "1", the second largest at 2, etc.

Lemma 3.2. *The value of*

$$z_1z_6 + z_2z_5 + z_3z_4, \tag{3}$$

is minimized under condition (2).

Proof. Without loss of generality, assume that $z_1 \geq z_i$ for any $2 \leq i \leq 6$. Supposing (for contradiction) that (2) does not hold, we have the following cases:

- If $z_6 > z_4$, consider the new system resulted from replacing Z_4 with Z_6 and Z_6 with Z_4. In the rest of this article, we will simply refer to this operation as "switching" the corresponding components. Now the new value for (3) is

$$z_1 z_4 + z_2 z_5 + z_3 z_6. \tag{4}$$

Comparing with the original value yields (4)-(3) as

$$z_1 z_4 - z_1 z_6 + z_3 z_6 - z_3 z_4 = (z_1 - z_3)(z_4 - z_6) \leq 0,$$

showing that the new system bears a value for (3) that is at most as large.

- Similarly, if $z_6 > z_5$, switching Z_6 and Z_5 yields the same conclusion.

- If $z_6 > z_2$ (or $z_6 > z_3$), switching Z_2 and Z_6 (or Z_3 and Z_6) will not increase the value (3). The calculation is similar and we leave it to the reader.

Now we may assume that $z_1 \geq z_i \geq z_6$ for any $2 \leq i \leq 5$. Focusing on z_i for $2 \leq i \leq 5$ and the value of $z_2 z_5 + z_3 z_4$, through similar argument, it is easy to see that (z_2, z_5) and (z_3, z_4) must be paired such that the largest (i.e., z_2) and smallest (i.e., z_5) values are paired together. $\square$

Remark 2. Note that (2) is a stronger condition than what we needed here but nevertheless minimizes (3).

For the second part of (1), we have the following through similar but slightly more complicated analysis.

Lemma 3.3. *The value of*

$$z_1z_2 + z_1z_3 + z_2z_4 + z_3z_5 + z_4z_6 + z_5z_6, \tag{5}$$

is maximized if and only if condition (2) *holds.*

Proof. Without loss of generality, assume that $z_1 \geq z_i$ for any $2 \leq i \leq 6$. Supposing that (2) does not hold:

- If $z_4 > z_2$, switching Z_2 and Z_4 yields a new value of (5) that is

$$z_1z_4 - z_1z_2 + z_2z_6 - z_4z_6 = (z_1 - z_6)(z_4 - z_2) \geq 0,$$

more than the original.

- If $z_4 > z_3$, switching Z_3 and Z_4, Z_5 and Z_6 (note that we are essentially “flipping” the portion $Z_3Z_5Z_6Z_4$) yields a new value of (5) that is at least as large. The calculation is similar and we leave it to the reader.

- Similarly, the cases for $z_5 > z_3$ or $z_5 > z_2$ can be handled in completely analogous way as the previous two cases.

- If $z_6 > z_2$ or $z_6 > z_3$, switching Z_2 and Z_6 or Z_3 and Z_6 will yield new systems with non-decreasing (5).

Now we can assume that $z_1 \geq z_2 \geq z_3 \geq \max\{z_4, z_5, z_6\}$. Following the same arguments, we have

- If $z_6 > z_4$, switch Z_4 and Z_6.

- If $z_6 > z_5$, switch Z_5 and Z_6.

Now we can assume that $z_1 \geq z_2 \geq z_3 \geq \max\{z_4, z_5\} \geq \min\{z_4, z_5\} \geq z_6$.

- If $z_5 > z_4$, switch Z_4 and Z_5.

Note that the value of (5) will strictly increase under the above assumptions and operations unless the corresponding z_i's are of the same value, we conclude that (2) is the necessary and sufficient condition to minimize (5). ☐

Lemmas 3.2 and 3.3 imply that the contribution $C(Z)$ from hexagonal edges are minimized when (2) holds for every hexagon. Together with Proposition 3.1, we have

Theorem 3.4. *With a given tree structure, the corresponding polyphenyl system has the minimum Wiener index if and only if condition* (2) *holds for every hexagon.*

Remark 3. Theorem 3.4 asserts that, with a given underlying tree structure, to minimize the Wiener index of the corresponding polyphenyl system one simply need to arrange the outgoing edges of every hexagon according to the size of the attached components (i.e., the values of z_i's).

With Theorem 3.4, one can easily check that Figure 6 provides a corresponding polyphenyl system that has the minimal Wiener index among all systems with the same underlying tree structure, i.e., Figure 8.

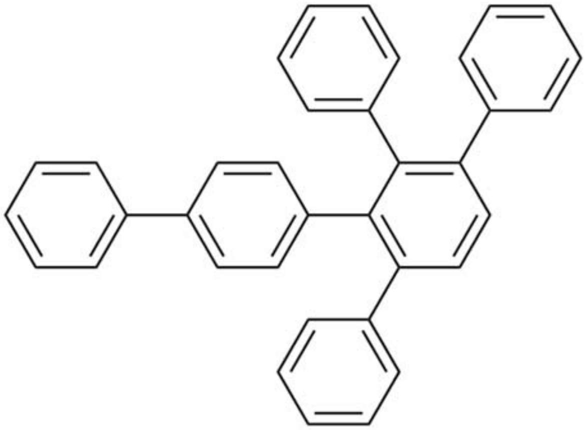

Figure 8. An extremal polyphenyl system that minimizes the Wiener index.

Remark 4. Although we focus our attention on the extremal structures in this section, our approach can be used to effectively compare the value of the Wiener indices of two isomeric tree-like polyphenyl systems even when they are not extremal. Examples of such application is shown in Section 5.

4. Between Adjacent Hexagons

In this section, we consider the influence, from interchanging pendant branches of two adjacent hexagons, on the Wiener index of a tree-like polyphenyl system. First note that for any two adjacent hexagons as in Figure 9, permuting any of the branches (with the possibility of being empty) $Z_{ij}(i = 1, 2 \text{ and } j = 1, 2, 3, 4, 5)$ will not affect the contribution to $C(Z)$ from any other hexagons except the two under consideration in Figure 9.

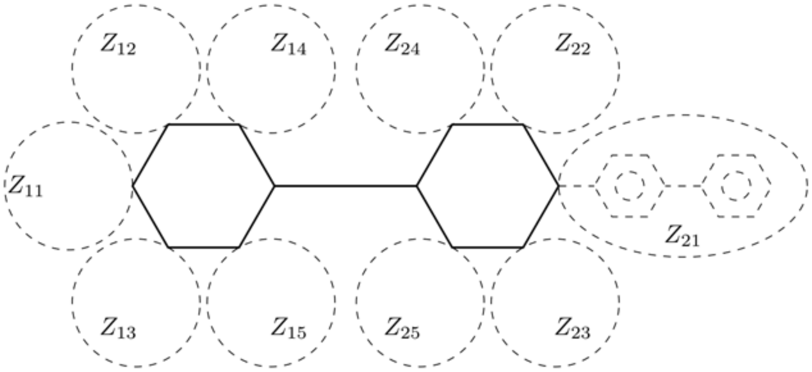

Figure 9. Adjacent hexagons and the resulting components.

This contribution (from this pair of adjacent hexagons) can be calculated similarly as that from Section 3 as:

$$\frac{5}{2}\left(\sum_{j=1}^{5} z_{1j} + \sum_{j=1}^{5} z_{2j}\right)^2 - \left(\sum_{j=1}^{5} z_{1j}^2 + \sum_{j=1}^{5} z_{2j}^2\right)$$

$$+ \sum_{i=1}^{2} (z_{i2}z_{i5} + z_{i3}z_{i4} - (z_{i1}z_{i2} + z_{i1}z_{i3} + z_{i2}z_{i4} + z_{i3}z_{i5}))$$

$$-\frac{3}{2}\left(\sum_{j=1}^{5} z_{1j}\right)^2 - \frac{3}{2}\left(\sum_{j=1}^{5} z_{2j}\right)^2$$

$$+ (z_{11} - z_{14} - z_{15})\left(\sum_{j=1}^{5} z_{2j}\right) + (z_{21} - z_{24} - z_{25})\left(\sum_{j=1}^{5} z_{1j}\right),$$

where $z_{ij} = |V(Z_{ij})|$.

Examining this expression, we have

(1) The first line

$$\frac{5}{2}\left(\sum_{j=1}^{5} z_{1j} + \sum_{j=1}^{5} z_{2j}\right)^2 - \left(\sum_{j=1}^{5} z_{1j}^2 + \sum_{j=1}^{5} z_{2j}^2\right),$$

is a constant.

(2) For any pair of adjacent hexagons in the system, one only needs to consider maximizing or minimizing the expression

$$f := \sum_{i=1}^{2} (z_{i2}z_{i5} + z_{i3}z_{i4} - (z_{i1}z_{i2} + z_{i1}z_{i3} + z_{i2}z_{i4} + z_{i3}z_{i5}))$$

$$-\frac{3}{2}\left(\sum_{j=1}^{5} z_{1j}\right)^2 - \frac{3}{2}\left(\sum_{j=1}^{5} z_{2j}\right)^2$$

$$+ (z_{11} - z_{14} - z_{15})\left(\sum_{j=1}^{5} z_{2j}\right) + (z_{21} - z_{24} - z_{25})\left(\sum_{j=1}^{5} z_{1j}\right).$$

(3) Repeating (2), one can continue to increase or decrease the expression of f for pairs of adjacent hexagons. Note that in every step the value of $W(Z)$ will be strictly increased or decreased. Hence this process terminates in finite steps.

Remark 5. In terms of the structural change of chemical compounds, the "switching" of Z_{ij}'s is merely breaking and forming bonds (ones that connect some Z_{ij} to one of the two hexagons). Among tree structures, it is known that a complete "chain decomposition" exists among the partially ordered set (ordered by the value of Wiener index) of trees of given order, where every pair of "adjacent" trees in a chain differ by only "breaking and forming" bonds at "adjacent locations". This offers an intuitive support for what is discussed above. Considering the same question on any pair of hexagons (not necessarily adjacent) follow from the same motivation, but the mathematical presentation would be rather tedious and much more technical.

5. Comparison with Physical Properties

In this section, we compare our theoretical studies with the predictions of physical properties of the following isomeric polyphenyls system (Figure 10). Details of these systems can be found in [1, 3, 4, 8, 10, 13, 14, 16, 17]. In what follows, we simply refer to them as A, B, C, D, E, and F.

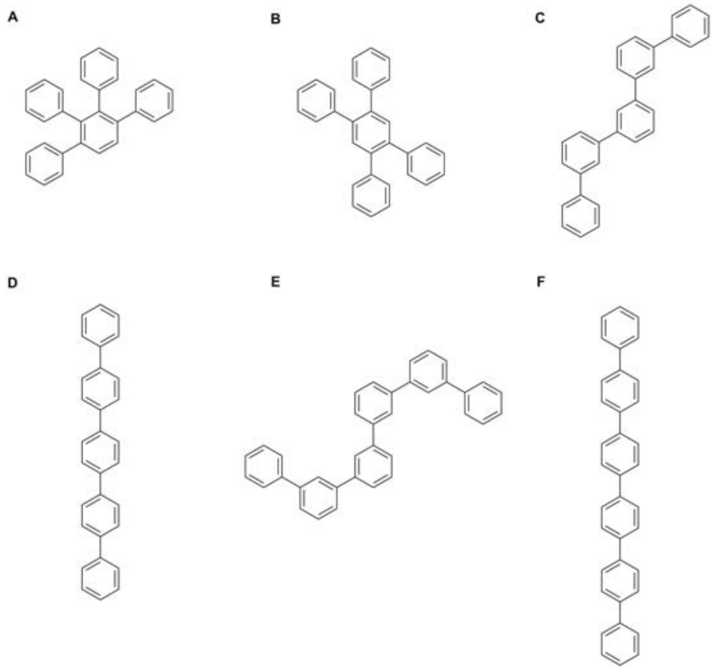

Figure 10. Polyphenyls with Wiener indices $W(A) = 2151$, $W(B) = 2223$, $W(C) = 2655$, $W(D) = 3015$, $W(E) = 4482$, and $W(F) = 5202$.

Also, A and B; C and D; and E and F are isomers (i.e., molecules with the same molecular formula, but different chemical structures) of each other. A, B, C, D are of the same size with 5 phenyl rings (pentaphenyl). E and F are 6 phenyl rings (hexaphenyl). Our discussions in Section 3 and Section 4 implies that

$$W(A) < W(B) < W(C) < W(D),$$

with A and D being the extremal cases that minimizes and maximizes the Wiener index, respectively.

Similarly, our discussion in Section 3 implies that

$$W(E) < W(F).$$

The following tables show some of the properties of these polyphenyls [25]. In particular, we see a clear correlation between the predicted boiling points, as well as enthalpy of vaporization and density, to the ordering according to the Wiener index. The Wiener indices can be efficiently calculated by using formulas such as (1).

Table 1. Predicted properties of polyphenyl compounds compared with the Wiener index (Data Provided from Advanced Chemistry Development Labs http://www.acdlabs.com)

Polyphenyls	Boiling Point (ºC at 760 Torr or 1 atm)	Wiener index
A	466.7 ± 40	2151
B	508.5 ± 45	2223
C	567.7 ± 30	2655
D	618.1 ± 35	3015
E	646.7 ± 40	4482
F	703.2 ± 45	5202

Remark 6. Note that there is naturally not any significant differences between densities (as can be seen in Table 2), however the clear correlation between the density and the Wiener index is still clearly presented here.

Table 2. Predicted properties of polyphenyl compounds compared with the Wiener index (Data Provided from Advanced Chemistry Development Labs http://www.acdlabs.com)

Polyphenyls	Enthalpy of Vaporization (kJ/mol)	Density	Wiener index
A	70.0 ± 0.8	1.091	2151
B	74.9 ± 0.8	1.091	2223
C	82.0 ± 0.8	1.091 ± 0.06	2655
D	88.3 ± 0.8	1.091 ± 0.06	3015
E	91.9 ± 0.8	1.102 ± 0.06	4482
F	99.2 ± 0.8	1.102 ± 0.06	5202

6. Concluding Remarks

In this article, we consider the Wiener index of tree-like polyphenyl systems. When the underlying tree structure is given, the extremal systems can be specifically characterized. When the systems have the same chemical molecular formula, but different structural arrangements (isomers) that possibly provides different tree structures, the study is more complicated. We provide a useful tool to study such systems by considering rearrangement of pendant branches of two adjacent hexagons. The computational results are also compared with predicted physical properties (such as boiling points, enthalpy of vaporization, and density) of these compounds. This study will help us to address systems that have all possible underlying tree structures.

It is known that among general tree structures of given order, the star (a tree where one vertex is adjacent to all other vertices) minimizes the Wiener index. From the discussion in Section 3, when a reduced tree structure is a star the contributions from non-hexagon edges to the Wiener index of a polyphenyl system is minimized. When the order of the reduced tree is at most 7, the star will indeed produce a feasible polyphenyl system.

As a first step of exploring the minimal Wiener index of such systems, trees with given order ≤ 7 and their corresponding polyphenyl systems can be explored through exactly the methods described in this article. Of particular importance is to note that proposed variations of the tree structure will change the value of (1) for each hexagon. Hence more in-depth study is needed.

A natural question would be that, is it true that, among tree-like polyphenyl systems of given order, the minimum (maximum) Wiener index is obtained when the underlying tree structure is extremal (with corresponding constraints such as maximum degree ≤ 6) and conditions such as (2) is satisfied.

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