

Generalized Wiener Indices in Hexagonal Chains

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Abstract

The Wiener Index, or the Wiener Number, also known as the “sum of distances” of a connected graph, is one of the quantities associated with a molecular graph that correlates nicely to physical and chemical properties, and has been studied in depth.

An index proposed by Schultz is shown to be related to the Wiener Index for trees, and Ivan Gutman proposed a modification of the Schultz index with similar properties.

We deduce a similar relationship between these three indices for catacondensed benzenoid hydrocarbons (graphs formed of concatenated hexagons, or hexagonal chains, or sometimes *acenes*). Indeed, we may define three *families* of Generalized Wiener Indices, which include the Schultz and Modified Schultz indices as special cases, such that similar explicit formulae for all Generalized Wiener Indices hold on hexagonal chains. We accomplish this by first giving a more refined proof of the formula for the standard Wiener Index of a hexagonal chain, then extending it to the Generalized Wiener Indices via the notion of partial Wiener Indices. Finally, we discuss possible extensions of the result.

1 Introduction

Chemists use many quantities associated with a molecular graph to estimate various physical properties. One of the eldest of these is the Wiener Index, defined in 1947 [34].

Definition 1 (Harold Wiener) *The Wiener Index of any connected graph G is defined as*

$$\mathcal{W}(G) := \sum_{\{u,v\} \subset V(G)} d_G(u,v).$$

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1.1 Some History Pertaining to Wiener Indices

The Wiener Index was first used by Wiener for approximating the boiling points of alkanes

$$\text{b.p.} \approx \alpha \mathcal{W}(G) + \beta w_3 + \gamma,$$

wherein α, β , and γ are empirical constants, and w_3 is the number of vertex pairs that are at distance 3 from each other in the molecular graph, called the “path number” by Wiener.

In general, the Wiener Index measures how compact a molecule is for its given weight. It therefore has predictive value and chemists and physics have found many such uses for the Wiener Index. Wiener Index thus has been studied in depth in the literature. We especially recommend the reference survey by Dobrynin, Entringer, and Gutman [5], which summarized the uses of the Wiener Index and all known efficient and elegant results on Wiener numbers of trees. The original publication of some of the best results are in [6, 21, 22].

Problems about Wiener Indices are still legion, and vary greatly in scopes and direction. Explicit formulas for the Wiener Indices (and its generalization to polynomials) of classes (or sequences) of graphs are sought, and properties are derived therefrom. Investigators also try to determine those natural numbers which Wiener Index can be attained for classes of graphs.

See final section also for other research directions. As mentioned in [5], there are different kinds of especially interesting problems regarding the Wiener Index for a given type of graphs:

- How the Wiener Index depends on the structure of the graph; particularly, which graphs of that type have the same Wiener Index.
- How to compute the Wiener Index efficiently (especially without needing a computer – the so-called “paper-and-pencil” methods); [6] is an excellent example of the latter.

Discussions around computing the Wiener Index of a generic chain-like polygonal system began from the late 1980’s [12, 13, 27]. Computing the Wiener Index for such a chain was once considered a very hard problem. To the best of our knowledge, the 1993 work in [18], involving studying incremental effects of the turns in a linear chain, represent the earliest explicit solution. The lack of clarity led to confusion, which was amended by several other works and authors.

The next year, the approach of studying the segments and the turns (sometimes named the “kinks”) was extended to giving the graphs of phenylenes and analogous graphs in [35, 36]. Other later better-written papers covered the same ground and more, and we recommend a look at [9, 19], as well as [17, 38], which covered a different type of polygonal structures.

Other notable investigators (not exhaustive) of the Wiener Index and representative work are: Balaban [25], Bonchev [1], Harary [2], Hosoya [15, 16], Merris [22], Mohar [24], Plesnik [26], Rouvray [29], Šoltés [32], Trinajstić [33]. Also see aforementioned Gutman [3, 11, 14].

1.2 The Schultz Index and Gutman’s Modification thereof

We first define the index S introduced by Schultz [31] and its modification S^* by Gutman [19].

Definition 2 ([19, 31]) *The Standard and Modified Schultz Index for a connected graph G are*

$$\begin{aligned} \mathcal{W}_+(G) := S(G) &:= \sum_{\{u,v\} \subset V(G)} (\deg_G u + \deg_G v) d_G(u, v). \\ \mathcal{W}_*(G) := S^*(G) &:= \sum_{\{u,v\} \subset V(G)} (\deg_G u \cdot \deg_G v) d_G(u, v). \end{aligned}$$

$\deg_G u$ is the degree of u in G (the number of first neighbors; this is often written as δ_u).

To avoid clutter and confusion, the modified Schultz Index proposed by Ivan Gutman (S^* or \mathcal{W}_*) will also be termed simply the *Modified Schultz Index*. The notation we choose here is intended to accentuate the relation between the indices. Indeed:

Theorem 1 ([7, 20]) *If G is a tree on n vertices (an n -tree)*

$$\begin{aligned}\mathcal{W}_+(G) &= 4\mathcal{W}(G) - n(n-1); \\ \mathcal{W}_*(G) &= 4\mathcal{W}(G) - (n-1)(2n-1).\end{aligned}$$

1.3 Our Goals Regarding the Schultz Indices

Almost all previous results on these indices have been about trees, but it is our goal to work with acenes (catacondensed benzenoid hydrocarbons) or rather their graphs, which are (unbranched) chains of concatenated hexagons and will be called *hexagonal chains*. These graphs have significance in connection with the phenylenes and hexagonal systems ([19], more references in [4, 40]). We shall prove this analogous theorem:

Theorem 2 *If G is an (unbranched) hexagonal chain composed of n fused hexagons, then*

$$\begin{aligned}\mathcal{W}_*(G) &= \frac{25}{4}\mathcal{W}(G) - \frac{3}{4}(2n+1)(20n+7). \\ \mathcal{W}_+(G) &= 5\mathcal{W}(G) - 3(2n+1)^2.\end{aligned}$$

En route to proving this result, we give in this paper explicit formulae for *all* Generalized Wiener Indices (which include the Schultz and Modified Schultz Indices) of hexagonal chains (acenes), extending the results in [18]. The results turn out to be surprisingly neat. We accomplish this by first giving a more refined proof of the formula for the standard Wiener Index of a hexagonal chain, then extending it to all Generalized Wiener Indices via the notion of partial Wiener Indices. We also obtain results on the effect of changing a segment and on the indices for hexagonal chains with periodic patterns. Further generalizations are discussed at last.

The rest of the paper is organized as follows. In Section 2 notations and preliminary results are given. In Section 3 we give a refined and more transparent proof of the formula for computing the standard Wiener Index of a hexagonal chain. In Section 4 we establish the main result, the formulae for computing Generalized Wiener Indices for a hexagonal chain. Subsidiary results and further generalizations are outlined in Section 5.

2 Preliminary

We give preliminary results that will be useful. First we set out our notations to describe a hexagonal chain. Let $n \in \mathbb{N}$ be a non-negative integer. Take the chain $P_{n+3} \times P_2$, which is $(n+2)$ squares connected edgewise together. Let $S \in \{0, 1, 2\}^n = (s_1, s_2, \dots, s_n)$ be a ternary n -string, we will add two points to each square making it into a hexagon such that the $(j+1)$ -th hexagon will have s_j vertices on the top row. We will denote by $H(S)$ this hexagonal chain.

A straight chain of $n+2$ hexes is $H(\overbrace{1 \cdots 1}^n)$, which we shorten to $H(1^n)$. See diagram (Fig. 1). We now introduce the *partial Wiener Indices*, which was first introduced in [18, 35, 37].

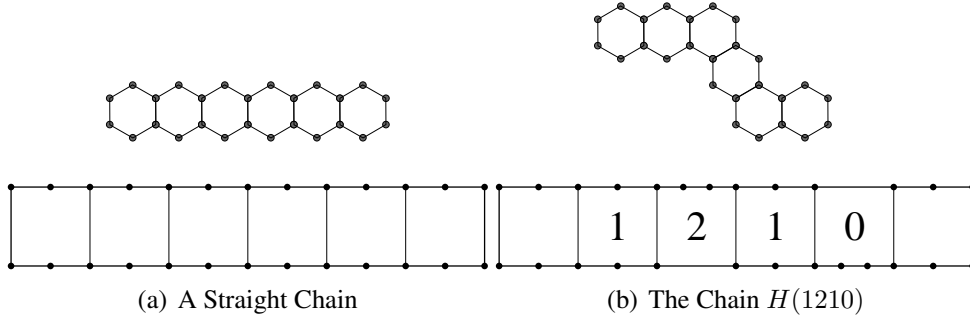


Figure 1: Two hexagonal chains (acenes) that contain six hexagons

Definition 3 For vertices $u \in V(G)$ or subsets of vertices $U \subset V(G)$:

$$\begin{aligned} \mathcal{W}(U, U'; G) &:= \sum_{u \in U, u' \in U'} d_G(u, u'), & \mathcal{W}(u, U; G) &:= \sum_{v \in U} d_G(u, v), \\ \mathcal{W}(U; G) &:= \sum_{\{u, u'\} \subset U} d_G(u, u'), & \mathcal{W}(u; G) &:= \sum_{v \in V(G)} d_G(u, v). \end{aligned}$$

These definitions are collectively called the *partial Wiener Indices* and encapsulate the information of distances between vertices or sets of vertices. It is then easy to prove the following basic result that we call the *Shelling Lemma*. This lemma is implicitly or explicitly invoked when proving most of the results pertaining to Wiener Indices and Polynomials ([35, 36]).

Lemma 3 ([18]) If $V(G) = U_1 \uplus U_2 \uplus \dots \uplus U_k$ (\uplus is disjoint union) then

$$\begin{aligned} \mathcal{W}(G) &= \sum_{j=1}^k \mathcal{W}(U_j; G) + \sum_{1 \leq i < j \leq k} \mathcal{W}(U_i, U_j; G) \\ &= \mathcal{W}(U_1; G) + \sum_{j=2}^k [\mathcal{W}((\uplus_{1 \leq i \leq j} U_i), U_j; G) - \mathcal{W}(U_j; G)]. \end{aligned}$$

The Divide-and-Conquer approach as seen in this lemma is often seen in combinatorics and other mathematical disciplines. The same idea will be used in Section 4 to prove the main results of this paper. A connected graph is called a *motley chain* [36] if it is formed by joining polygons at edges such three (or more) polygons do not intersect at any vertex. The following observation is crucial to computing the indices of Schultz and Gutman for motley chains.

Lemma 4 Let G be any motley chain,

$$\mathcal{W}_1(G) := \mathcal{W}(V_2, V_3; G), \quad \mathcal{W}_2(G) := \mathcal{W}(V_2; G), \quad \mathcal{W}_3(G) := \mathcal{W}(V_3; G),$$

where V_2 and V_3 are the sets of degree-2 and -3 vertices, then

$$\mathcal{W} = \mathcal{W}_1 + \mathcal{W}_2 + \mathcal{W}_3, \quad \mathcal{W}_+ = 5\mathcal{W}_1 + 4\mathcal{W}_2 + 6\mathcal{W}_3, \quad \mathcal{W}_* = 6\mathcal{W}_1 + 4\mathcal{W}_2 + 9\mathcal{W}_3. \quad (1)$$

Proof. We merely have to observe that motley chains only has vertices of degrees 2 and 3, and this lemma follows immediately from the shelling lemma. \square

In fact, we accomplish much more. We will consider these three families of variations on Wiener Indices, which include the Schultz and Modified Schultz indices as special cases.

Definition 4 For a connected graph G , define families of generalized Wiener Indices of G by

$$\begin{aligned}\mathcal{W}_{\ddagger}^{(\alpha)}(G) &:= \sum_{\{u,v\} \subset V(G)} ((\deg_G u)^\alpha + (\deg_G v)^\alpha) d_G(u,v). \\ \mathcal{W}_{+}^{(\alpha)}(G) &:= \sum_{\{u,v\} \subset V(G)} (\deg_G u + \deg_G v)^\alpha d_G(u,v). \\ \mathcal{W}_{*}^{(\alpha)}(G) &:= \sum_{\{u,v\} \subset V(G)} (\deg_G u)^\alpha (\deg_G v)^\alpha d_G(u,v).\end{aligned}$$

Other generalizations (i.e., Randić [28]) of the Wiener Index have been proposed, but from now on we will collectively term the above quantities *Generalized Wiener Indices*, in contrast to the (standard) Wiener Index. We may see that analogously to Lemma 4, we have

Lemma 5 For any motley chain, we have

$$\begin{aligned}\mathcal{W}_{\ddagger}^{(\alpha)} &= (2^\alpha + 3^\alpha)\mathcal{W}_1 + 2 \cdot 2^\alpha \mathcal{W}_2 + 2 \cdot 3^\alpha \mathcal{W}_3, \\ \mathcal{W}_{+}^{(\alpha)} &= 5^\alpha \mathcal{W}_1 + 4^\alpha \mathcal{W}_2 + 6^\alpha \mathcal{W}_3, \\ \mathcal{W}_{*}^{(\alpha)} &= 6^\alpha \mathcal{W}_1 + 4^\alpha \mathcal{W}_2 + 9^\alpha \mathcal{W}_3.\end{aligned}$$

3 The Standard Wiener Index for a Hexagonal Chain

In this section we will give a more direct and transparent proof of the [18] formula for computing $\mathcal{W}(H(S))$ for an arbitrary string S . However, the technique we present gives much more than just an improvement on an old proof, because it will generalize to proving a similar formula about the Generalized Wiener Indices in the next section.

The strategy is to compare the string S with the string 1^n . The Wiener Index of $H(1^n)$ may have been found independently more than once [12], and can be proved by induction.

Proposition 6 The Wiener Index for $H(1^n)$ is

$$\mathcal{W}(H(1^n)) = (16n^3 + 132n^2 + 362n + 327)/3. \quad (2)$$

We define the following notation to record the turning positions of a hexagonal chain.

Definition 5 Let $S = s_1 s_2 \cdots s_n \in \{0, 1, 2\}^n$ be a n -string, we define

$$\begin{aligned}B = B_S &:= \{j \in \{1, 2, \dots, n\} : s_j \neq 1\}, \\ \bar{j} = \bar{j}_S &:= \begin{cases} \min\{i \in B_S : i > j\}, & \text{if } \{i \in B_S : i > j\} \neq \emptyset, \\ n + 1, & \text{otherwise;} \end{cases} \\ C = C_S &:= \{j \in B_S : \{i \in B_S : i > j\} \neq \emptyset, s_j = s_{\bar{j}_S}\}.\end{aligned}$$

We can think of the ternary digit 1 as going straight, B marks the ‘‘bent’’ positions and C marks the ‘‘curled’’ positions, having two bends go the same way. Given these definitions, $\mathcal{W}(H(S))$ is computed as follows. This result encompasses all previous ones in [12, 13, 27].

Theorem 7 *Let the notations be defined above, then*

$$\Delta\mathcal{W}(H(S)) := \mathcal{W}(H(S)) - \mathcal{W}(H(1^n)) = 8 \left[\sum_{j \in B_S} j(\bar{j}_S - j) + 2 \sum_{j \in C_S} j(n+1 - \bar{j}_S) \right]. \quad (3)$$

Proof. Let $B = B_S = \{j_1 < j_2 < \dots < j_k\}$. We define a sequence of strings $S := S_0, S_1, \dots, S_k := 1^n$, such that S_{i-1} is equal to S_i except in the j_i -th position, where the original 0 or 2 is replaced by 1. For example, if $S = 1210$ then $S_2 = S, S_1 = 1110, S_0 = 1111$.

Clearly, $\Delta\mathcal{W}(S) = \sum_{i=1}^k (\mathcal{W}(H(S_i)) - \mathcal{W}(H(S_{i-1})))$. We can see $H(S_i)$ as comprising j_i straight hexes, then the turning hex, then a further $j_{i+1} - j_i$ straight hexes, then bending to the remaining $n+1 - j_{i+1}$ hexes which are not necessarily straight.

We may define $j_{k+1} := n+1$ to take care of the boundary case, then for each i ,

$$\mathcal{W}(H(S_i)) - \mathcal{W}(H(S_{i-1})) = \begin{cases} 8j_i(j_{i+1} - j_i) + 16j_i(n+1 - j_{i+1}), & \text{if } j_i \in C_S, \\ 8j_i(j_{i+1} - j_i), & \text{if } j_i \notin C_S. \end{cases}$$

This claim implies Eq. 3. To prove it, use the shelling lemma and writes

$$\begin{aligned} \mathcal{W}(H(S)) &= \mathcal{W}(\text{right side}; H(S)) + \mathcal{W}(\text{left side}; H(S)) + \mathcal{W}(\text{turning hex}; H(S)) \\ &+ \mathcal{W}(\text{turning hex, right side}; H(S)) + \mathcal{W}(\text{turning hex, left side}; H(S)) \\ &+ \mathcal{W}(\text{left side, right side}; H(S)) \end{aligned} \quad (4)$$

When we straighten out the turn at some hex, only the last term of Eq. 4 changes.

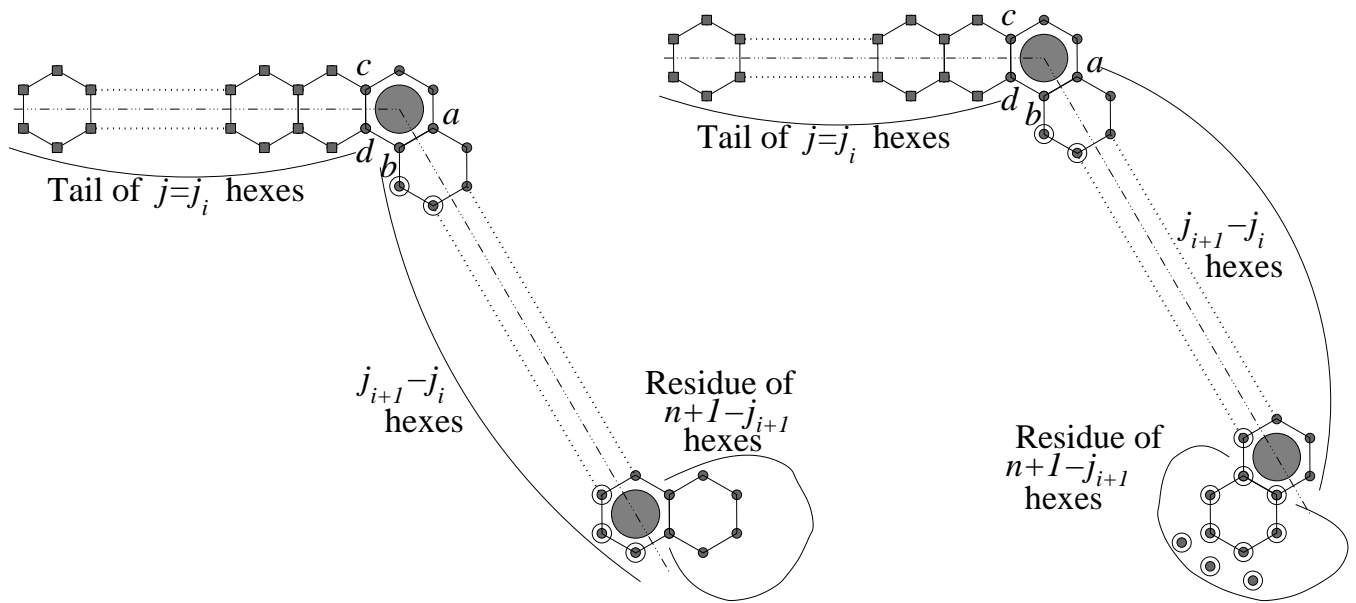
If we look at the right side of the turning hex, everything above the dotted line has a shortest path to the ‘‘tail’’ (marked as squares) on the left through the vertex a . As we straighten the ‘‘bend’’, a moves to a' with the entire upper-right portion following in its steps. But a and a' are symmetric respective to the tail, i.e., the distance of any vertex in the lower half of the tail (behind d) to a' is one more than to a , but the distance of any vertex in the upper half of the tail (behind c) correspondingly is one less than to a' than to a , so all this cancels out and contributes no change to the Wiener Index.

In contrast, b moves to b' , which is not equi-distant to the tail on the left. Indeed, b' is one further away than b from either c or d , and hence from each of the $4j_i$ vertices in the tail. The same applies to each vertex below the dotted line on the right (vertices marked by circles). There are $2(j_{i+1} - j_i)$ such vertices in the straight segment, two in each hex. Further, when and only when this bend position is followed by another turn in the same direction — i.e., this is an index in C_S — do the remaining $n+1 - j_{i+1}$ hexes (with 4 vertices to a hex) belong to this group as well. We have proved the claim and hence the proposition. \square

Corollary 7.1 ([12]) *For the same number of hexes, the largest and smallest Wiener Indices are attained at straight ($H(1^n)$) and the coiled chain $H(0^n)$ (or equivalently $H(2^n)$).*

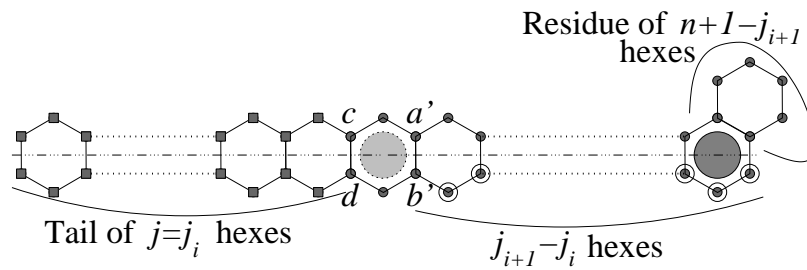
4 Generalized Wiener Indices of a Hexagonal Chain

We now compute all Generalized Wiener Indices of a hexagonal chain.

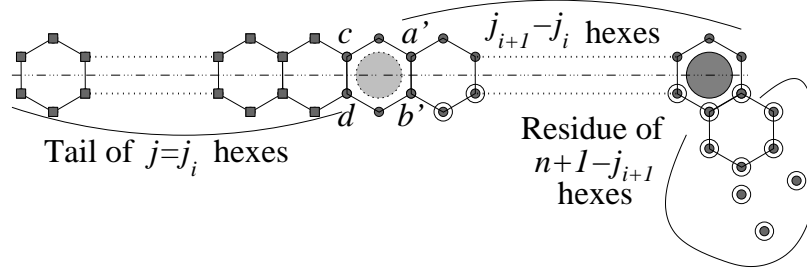


(a) Before Straightening (Case $B - C$)

(b) Before Straightening (Case C)



(c) After Straightening (Case $B - C$)



(d) After Straightening (Case C)

Note that as we straighten out the turn at some hex, only distances between the right (residual) and left (tail) sides can change; i.e. only the last term of Eq. 4 changes.

Figure 2: As we straighten out the turning at location j_i

Theorem 8 Let $\widehat{\mathcal{W}}$ denote any of the indices above, then for any string $S \in \{0, 1, 2\}^n$

$$\widehat{\mathcal{W}}(H(S)) = \widehat{\mathcal{W}}(H(1^n)) - \widehat{a} \left[\sum_{j \in B(S)} j(\bar{j}_S - j) + 2 \sum_{j \in C(S)} j(n + 1 - \bar{j}_S) \right]. \quad (5)$$

Where the coefficient \widehat{a} is equal to 8 for the standard Wiener Index \mathcal{W} , 40 for \mathcal{W}_+ , 50 for \mathcal{W}_* , $8 \cdot (2^\alpha + 3^\alpha)$ for $\mathcal{W}_\ddagger^{(\alpha)}$, $8 \cdot 6^\alpha + 2 \cdot (3^\alpha - 2^\alpha)^2$ for $\mathcal{W}_*^{(\alpha)}$, and $2 \cdot 6^\alpha + 4 \cdot 5^\alpha + 2 \cdot 4^\alpha$ for $\mathcal{W}_+^{(\alpha)}$.

Corollary 8.1 Any two hexagonal chains of the same length has \mathcal{W}_+ and \mathcal{W}_* that differ by multiples of 40 and 50 respectively. Indeed, any given Generalized Wiener Index $\widehat{\mathcal{W}}$ will differ on two equally long chains by a multiple of its \widehat{a} (which is 8 for the original Wiener Index).

By Lemma 4 we only need to take care of \mathcal{W}_2 and \mathcal{W}_3 , and there is no need to consider \mathcal{W}_1 , since $\mathcal{W} = \mathcal{W}_1 + \mathcal{W}_2 + \mathcal{W}_3$. Therefore Theorem 8 is an immediate corollary of the following:

Lemma 9 For any string $S \in \{0, 1, 2\}^n$:

$$\begin{aligned} \mathcal{W}_2(H(1^n)) - \mathcal{W}_2(H(S)) &= \mathcal{W}_3(H(1^n)) - \mathcal{W}_3(H(S)) \\ &= \frac{1}{4} \mathcal{W}(H(1^n)) - \mathcal{W}(H(S)) = 2 \left[\sum_{j \in B(S)} j(\bar{j}_S - j) + 2 \sum_{j \in C(S)} j(n + 1 - \bar{j}_S) \right]. \end{aligned} \quad (6)$$

Proof. We draw Fig. 2 again with deg-3 vertices in black and deg-2 vertices in white.

First we find $\Delta\mathcal{W}_3$. In computing $\Delta\mathcal{W}$ earlier in Theorem 7, the turning hex itself does not change and hence contributes no change in the Wiener Index. For \mathcal{W}_3 , we see that

- any vertex behind a does not change distance to the tail as we straighten the turn.
- for any deg-3 vertex behind b (circled white vertices), its distance to each of the $(2j_i)$ deg-3 vertices in the tail (white squares) increases by one when we straighten the turn.
- There is one circled white vertex for each of the $j_{i+1} - j_i$ hexes in the straight segment following the turn and, *if and only if there are two consecutive turns in the same direction, i.e., a C position, two more for each of the remaining $n + 1 - j_{i+1}$ hexes.*

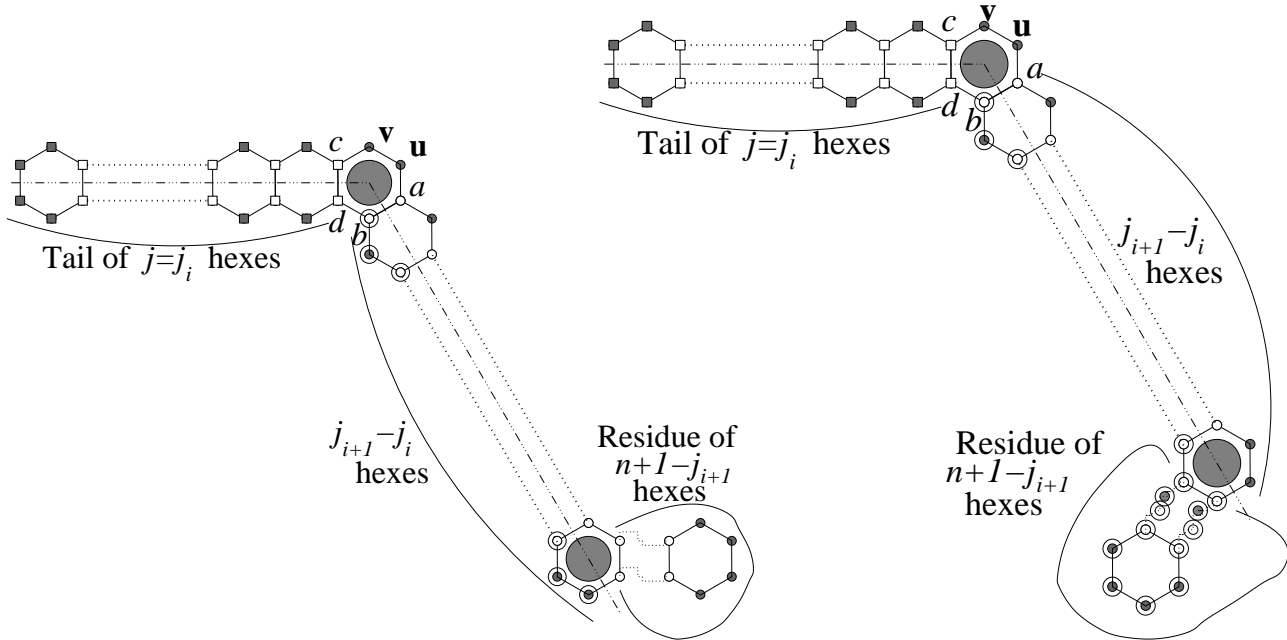
Thus, the second half (about \mathcal{W}_3) of Eq. 6 is proved. Now to prove the first half about \mathcal{W}_2 , and we will again use the shelling lemma and track the changes in each category:

$$\begin{aligned} \mathcal{W}_2(H(S)) &= \mathcal{W}_2(\text{right side}; H(S)) + \mathcal{W}_2(\text{left side}; H(S)) + \mathcal{W}_2(\text{turning hex}; H(S)) \\ &+ \mathcal{W}_2(\text{turning hex, right side}; H(S)) + \mathcal{W}_2(\text{turning hex, left side}; H(S)) \\ &+ \mathcal{W}_2(\text{left side, right side}; H(S)) \end{aligned} \quad (7)$$

So straightening out the turn at location j_i creates the following differences:

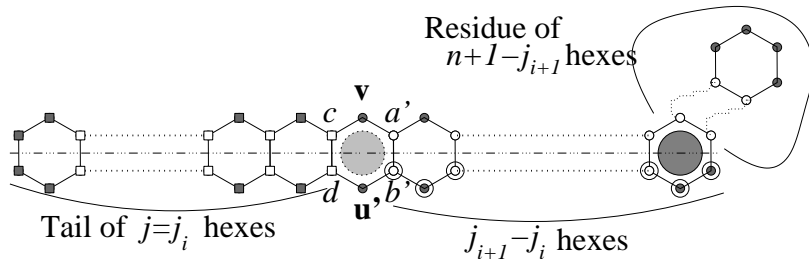
Within the left side and within the right side: no change.

The turning hex: +2, as $d(u, v) = 3$ in diagrams (a) and (c), $d(u', v) = 1$ in (b) and (d).

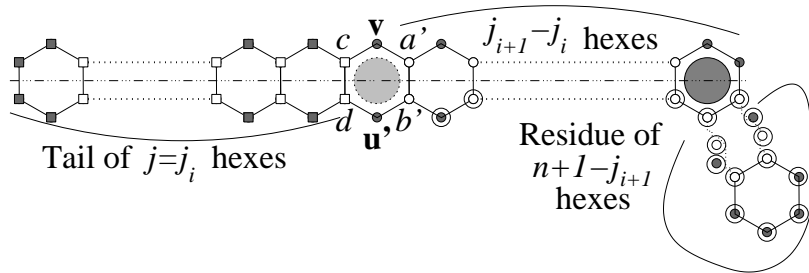


(a) Before Straightening (Case B – C)

(b) Before Straightening (Case C)



(c) After Straightening (Case B – C)



(d) After Straightening (Case C)

Please compare with Fig. 2 and observe the similar but slightly different patterns of change.

Figure 3: Changes in \mathcal{W}_2 and \mathcal{W}_3 as we straighten out a turn position

From the turning hex to the left side: none for vertices behind c ; -2 for each deg-2 vertex behind d (black squares in the lower half of the tail), of which there are $(j_i + 1)$.

From the turning hex to the right side: No change for vertices behind a (upper half of the residue), that is, $d(a, u) + d(a, v) = d(a', u') + d(a', v) = 3$, -2 for each vertex behind b (circled black vertices), because $d(b, u) + d(b, v) = 5$, $d(b', u') + d(b', v) = 3$.

Between the left and the right sides: $+1$ for each deg-2 vertex on the lower half of the right side (circled black vertices) and each of the deg-2 vertex in the tail (black squares).

So if the deg-2 (black) vertices behind b (circled) number n_b , then we have a total change of

$$2 - 2(j_i + 1) - 2n_b + 2(j_i + 1)n_b = 2(n_b - 1)((j_i + 1) - 1) = 2j_i \cdot (n_b - 1).$$

What is this n_b ? We need to look at the $B - C$ case and the C case separately. Normally, each hex of the straight section following the turn will have one vertex of degree 2 under the (dotted) center line. However, in the first ($B - C$) case, the last hex of the straight section has an extra deg-2 vertex, so $n_b = j_{i+1} - j_i + 1$. For the latter (C) case, the last hex of the straight section would be missing that black circled vertex. However, there will be *two* vertices of degree 2 in each of the remaining $n + 1 - j_{i+1}$ hexes, plus 2 extras at the end, each of which will be under the center line. So $n_b = [(j_{i+1} - j_i - 1) + 2(n + 1 - j_{i+1}) + 2]$, and

$$\mathcal{W}_2(H(S_{i+1})) - \mathcal{W}_2(H(S_i)) = \begin{cases} 2j_i \cdot (j_{i+1} - j_i), & j_i \in B_S - C_S; \\ 2j_i \cdot (j_{i+1} - j_i) + 4j_i \cdot (n + 1 - j_{i+1}), & j_i \in C_S. \end{cases}$$

We have proved all of Eq. 6 and the theorem. \square

As applications we turn back to Generalized Wiener Indices. First we need the base values $\mathcal{W}_2(H(1^n))$ and $\mathcal{W}_3(H(1^n))$. The proof is trivial by mathematical induction.

Lemma 10 *For straight hexagonal chains $(n + 2)$ -long we have*

$$\mathcal{W}_2(H(1^n)) = (4n^3 + 51n^2 + 194n + 228)/3; \quad \mathcal{W}_3(H(1^n)) = (4n^3 + 15n^2 + 14n + 3)/3. \quad (8)$$

Now combining $\mathcal{W}_+ = 5\mathcal{W} + \mathcal{W}_3 - \mathcal{W}_2$, $\mathcal{W}_* = 6\mathcal{W} + 3\mathcal{W}_3 - 2\mathcal{W}_2$ and Theorem 8, after a simple calculation we obtain Theorem 2, or we can write down the explicit formulae for computing the Generalized Wiener indices of Schultz and Gutman for hexagonal chains:

Corollary 10.1 *For n -long ternary S*

$$\begin{aligned} \mathcal{W}_+(H(S)) &= \frac{80n^3 + 624n^2 + 1756n + 1410}{3} - 40 \left[\sum_{j \in B(S)} j(\bar{j}_S - j) + 2 \sum_{j \in C(S)} j(n + 1 - \bar{j}_S) \right]; \\ \mathcal{W}_*(H(S)) &= \frac{100n^3 + 735n^2 + 1826n + 1515}{3} - 50 \left[\sum_{j \in B(S)} j(\bar{j}_S - j) + 2 \sum_{j \in C(S)} j(n + 1 - \bar{j}_S) \right]. \end{aligned}$$

Corollary 10.2 *For the same number of hexes, the largest and smallest Generalized Wiener Indices are attained at straight $(H(1^n))$ and the chain $H(0^n)$ (or equivalently $H(2^n)$).*

Corollary 10.3 For hexagonal chains, any Generalized Wiener Index $\widehat{\mathcal{W}}$ satisfy the relation

$$\widehat{\mathcal{W}} = \widehat{a}\mathcal{W} + p(n),$$

where \widehat{a} is as in Theorem 8 and p is a quadratic polynomial in n , the number of hexagons. Thus, we obtain explicit formulas easily for any Generalized Wiener on hexagonal chains.

This section also represent methods for effective computations, “paper-and-pencil methods”, of a little practical interest. Similarly for the results in the following section.

5 Discussions

We have shown how to compute all other Generalized Wiener Indices (including the Schultz and Modified Schultz Indices), for hexagonal chains. We discuss some further results and future directions below.

5.1 More Results Extended to Generalized Wiener Indices

There are several subsidiary results about the Wiener Index on a hex chain that can be extended directly using Theorem 8 and Corollary 10.1 to any given Generalized Wiener Index $\widehat{\mathcal{W}}$. We list two results in the following and the proofs are omitted since they are similar to that in [18].

The first theorem discusses the effect when we change a segment of the string.

Theorem 11 Suppose in the string $S \in \{0, 1, 2\}^n$, the digits s_i, \dots, s_j may vary, and $s_h \neq s_{h+1} = \dots = s_{i-1} = 1, 1 = s_{j+1} = \dots = s_{k-1} \neq s_k$,

If $s_h = s_k$: The minimum $\widehat{\mathcal{W}}$ is always at $s_h = s_i = s_{i+1} = \dots = s_j = s_k$. If we let

$$y_1 := 2h(2n + 2 - h - k), \quad y_2 := h(i - h) + i(k - i), \quad y_3 := h(j - h) + j(k - j);$$

$$\text{then } \max \widehat{\mathcal{W}} \text{ happens at } \begin{cases} s_i = s_{i+1} = \dots = s_j = 1, & \text{if } y_1 \leq y_2, y_3; \\ s_i = 2 - s_h, s_{i+1} = \dots = s_{j-1} = s_j = 1, & \text{if } y_2 \leq y_1, y_3; \\ s_i = s_{i+1} = \dots = s_{j-1} = 1, s_j = 2 - s_k, & \text{if } y_3 \leq y_1, y_2. \end{cases}$$

The difference between maximum and minimum is $\widehat{a} \cdot (\mathcal{W}_d - \min(y_1, y_2, y_3))$, where \widehat{a} is the coefficient corresponding to $\widehat{\mathcal{W}}$ in Theorem 8, and

$$\mathcal{W}_d = h(2n + 2 - h - i) + j(2n + 2 - j - k) + (2n - 1) \left[\binom{j}{2} - \binom{i}{2} \right] - 4 \left[\binom{j}{3} - \binom{i}{3} \right].$$

If $s_h \neq s_k$: The maximum $\widehat{\mathcal{W}}$ is always at $s_i = s_{i+1} = \dots = s_j = 1$. If we let

$$y_4 := h(n + 1 - i), \quad y_5 := j(n + 1 - k),$$

$$\text{then } \min \widehat{\mathcal{W}} \text{ happens at } s_i = s_{i+1} = \dots = s_j = \begin{cases} s_h, & \text{if } y_4 \geq y_5; \\ s_k, & \text{if } y_5 \geq y_4. \end{cases}$$

The difference between maximum and minimum is $8(\mathcal{W}_d - 2 \min\{y_4, y_5\} - h(k - h))$.

The second set of results considers the cases when the string S is periodic.

Theorem 12 Given $S \in \{0, 1, 2\}^n$, $S \neq 1^n$ and $m > 0$, we have:

$$\begin{aligned} \frac{\widehat{\mathcal{W}}(H(1^{mn})) - \widehat{\mathcal{W}}(H(S^m))}{\widehat{a}} &= -(s_b - 1)(s_{b'} - 1)(n - b')(b - 1) \\ &+ m \left[2 \sum_{j \in \bar{C}} j(n + 1 - \bar{j}) + \sum_{j \in B} j(\bar{j} - j) + (s_b - 1)(s_{b'} - 1)(b - 1)n \right] \\ &+ \binom{m}{2} \left[n^2 - 2n \sum_{j \in \bar{C}} (\bar{j} - j) + 2n|\bar{C}|(n + 1) \right] + \binom{m}{3} (2n^2|\bar{C}|), \end{aligned} \quad (9)$$

Here \widehat{a} , B , C , \bar{j} is defined as above, and

$$\begin{aligned} b &= \min B_S, & \bar{C} &= \begin{cases} C_S \cup \{b'\}, & \text{if } s_b = s_{b'}, \\ C_S, & \text{else;} \end{cases} \\ b' &= \max B_S, & \bar{j} &= \begin{cases} \bar{j}, & \text{if } j < b', \\ n + b, & \text{else.} \end{cases} \end{aligned}$$

The probabilistic results [13, 35] can of course be generalized as well for any $\widehat{\mathcal{W}}$.

5.2 Generalizations of Wiener (Hosoya) Polynomials and Future Work

Hosoya [16] introduced the following generating function of distance (a q -analogue to the Wiener Index) which he termed the Wiener Polynomial. Today, it is most frequently referred to as the Hosoya Polynomial, but we retain the original name to show the parallel:

$$H(G; q) := \mathcal{W}(G, q) := \sum_{\{u,v\} \subset V(G)} q^{d_G(u,v)}$$

Later, Sagan and Yeh [30] showed the absolute Poincare polynomials of Coxeter groups to be equal to the Wiener polynomial of its induced graph. Little was known about properties of the Wiener Polynomials of a general graph. Finding Wiener Polynomials explicitly can be difficult, for example, it was only recently solved for the polygonal chains [39], see also [37, 10].

There is a way to combine all the above concepts in a multivariate generating function, e.g.:

Definition 6 For subsets of vertices $U, U' \in V(G)$, define these trivariate polynomials:

$$\begin{aligned} \mathcal{W}(G; q, x, y) &:= \frac{1}{2} \sum_{u,v \in V(G)} q^{d_G(u,v)} x^{\deg_G u} y^{\deg_G v}, \\ \mathcal{W}(U, U'; G; q, x, y) &:= \sum_{u \in U, u' \in U'} q^{d_G(u,u')} x^{\deg_G u} y^{\deg_G u'}, \end{aligned}$$

and similar items analogously. We call them the *Generalized Multivariate Wiener Polynomials*.

Obviously, we can specialize the above to polynomials of Hosoya and Gutman [8]:

$$\begin{aligned} H(G; q) &:= \mathcal{W}(G, q) := \sum_{\{u,v\} \subset V(G)} q^{d_G(u,v)} = \mathcal{W}(G; q, 1, 1) \\ H_1(G; q) &:= \mathcal{W}_+(G; q) := \sum_{\{u,v\} \subset V(G)} (\deg_G u + \deg_G v) q^{d_G(u,v)} = \left. \frac{\partial}{\partial x} \mathcal{W}(G; q, x, x) \right|_{x=1} \\ H_2(G; q) &:= \mathcal{W}_*(G; q) := \sum_{\{u,v\} \subset V(G)} (\deg_G u \cdot \deg_G v) q^{d_G(u,v)} = \left. \frac{\partial^2}{\partial x \partial y} \mathcal{W}(G; q, x, y) \right|_{x=y=1} \end{aligned}$$

Indeed, we can create entire sequences of Generalized Wiener Polynomials $\mathcal{W}_{\ddagger}^{(\alpha)}(G; q)$, $\mathcal{W}_{+}^{(\alpha)}(G; q)$, $\mathcal{W}_{*}^{(\alpha)}(G; q)$ similarly (this is also possible for other multivariate generating functions). E.g.:

$$\mathcal{W}_{+}^{(\alpha)}(G; q) := \sum_{\{u,v\} \subset V(G)} (\deg_G u + \deg_G v)^{\alpha} q^{d_G(u,v)} = \left[\left(x \frac{\partial}{\partial x} \right)^{\alpha} \mathcal{W}(G; q, x, x) \right]_{x=1}.$$

Wiener Polynomials of hexagonal chains are given by [37, 39]. Of course, they are much more complex than for Wiener Index. There are still much to be studied about such distance-based polynomials (generating functions). For example, Gutman [8] proved an affine relation between $\mathcal{W}_{+}(G; q)$ or $\mathcal{W}_{*}(G; q)$ and $\mathcal{W}(G; q)$ on an n -tree:

$$\begin{aligned} \mathcal{W}_{+}(G; q) &= 2 \left(1 + \frac{1}{q} \right) \mathcal{W}(G; q) - 2 \left(1 + \frac{n}{q} \right) \\ \mathcal{W}_{*}(G; q) &= \left(1 + \frac{1}{q} \right)^2 \mathcal{W}(G; q) - \left(1 + \frac{1}{q} \right) \left(1 + \frac{2}{q} \right) n + \left(1 + \frac{1}{q} \right) + \sum_{x \in V(G)} (\deg_G x)^2 \end{aligned}$$

We note the following possibilities for future work in this area:

- A similar affine relationship may exist between Wiener Polynomials and the Generalized Wiener Polynomials on hexagonal chains.
- An affine relationship does *not* exist between the Standard and Generalized Wiener Indices (either the Schultz or Modified Schultz Index) on pentagonal chains.
- However, it may still be possible as a parallel of this paper to compute an explicit formula for any Generalized Wiener Index on a pentagonal chain (analogous to [35]).
- It may also be possible to compute explicit formulas for the Generalized Wiener Indices or Polynomials on other motley chain graphs (as in [36, 37, 39]) in general.

In other words, there are still a rich class of open problems for which combinatorial solutions are yet to be found, some of which may be very interesting mathematically or chemically.

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References

- [1] D. Bonchev, *Information theoretic indices for characterization of chemical structure*, Research Studies Press(Chichester), 1983.
- [2] F. Buckley and F. Harary, *Distances in Graphs*, Addison-Wesley (New York), 1990.
- [3] J.-C. Chen, I. Gutman and Y.-N. Yeh, *On the sum of all distances in graphs*, Tamkang J. of Mathematics 25(1993), 83–86.

- [4] V. Chepoi and S. Klavžar, *Distances in benzenoid systems: Further developments*, Disc. Math. 192 (1998) 27–39.
- [5] A. Dobrynin, R. Entringer, I. Gutman, *Wiener Index of Trees: Theory and Applications*, Acta Appl. Math. 66 (2001) 211–249.
- [6] I. Gutman, *A Formula for the Wiener Number of Trees and its Extension to Graphs Containing Cycles*, Graph Theo. Notes 27 (1994), 9–15.
- [7] I. Gutman, *Selected Properties of the Schultz molecular topological index*, J. Chem. Info. Comput. Sci. 34 (1994), 1087–1089.
- [8] I. Gutman, *Some Relations between distance-based polynomials of trees*, to appear.
- [9] I. Gutman, and S. Klavžar: *Relations between Wiener numbers of benzenoid hydrocarbons and phenylenes*, ACH Models Chem. 135 (1998), 45–55.
- [10] I. Gutman, S. Klavžar, M. Petkovaek, and P. Žigert, *On Hosoya polynomials of benzenoid graphs*, Comm. Math. Comp. Chem. (MATCH) 43 (2001), 49–66.
- [11] I. Gutman and O. E. Polansky, *Mathematical concepts in organic chemistry*, Springer-Verlag (Berlin), 1986
- [12] I. Gutman, *Wiener numbers of benzenoid hydrocarbons: Two theorems*, Chem. Phys. Letters, 136 (1987) 134–136.
- [13] I. Gutman, J. W. Kennedy and L. V. Quintas, *Wiener numbers of random benzenoid chains*, Chemical Physics Letters, 173 (1990) 403–408.
- [14] I. Gutman and Y.-N. Yeh, *On the sum of all distances in composite graphs*, Disc. Math. 135 (1994), no. 1–3, 359–365.
- [15] H. Hosoya, *Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons*, Bull. Chem. Soc. Jpn. 44(1971), 2332–2339.
- [16] H. Hosoya, *On some counting polynomials in Chemistry*, Disc. Appl. Math. 19 (1988), 239–257.
- [17] I-W. Huang, B.-Y. Yang, and Y.-N. Yeh, *Wiener Indices of Hex Carpets— from Hexagon Models to Square Grids*, SE Asia Bull. of Math. 20 (1996), 81–102.
- [18] W.-C. Huang, B.-Y. Yang, and Y.-N. Yeh, *From Ternary Strings to Wiener indices of Benzenoid Chains*, Disc. Appl. Math. 73 (1997), 113–131.
- [19] S. Klavžar and I. Gutman, *Wiener number of vertex-weighted graphs and a chemical application* Disc. Appl. Math. 80 (1997), 73–81.
- [20] D. J. Klein, Z. Mihalić, D. Placšić, and N. Trinajstić, *Molecular topological index: a relation with the Wiener index*, J. Chem. Info. Comput. Sci. 32 (1992), 304–305.
- [21] S.-C. Liu, L.-D. Tung, and Y.-N. Yeh, *The Trees with Minimum Wiener Number*, Intl. J. of Quant. Chem., 78(2000), 331–340.
- [22] R. Merris, *Laplacian Matrices of Graphs: a Survey*, Linear Alg. Appl. 197/198 (1994), 143–176.

- [23] R. Merris, *An edge version of the matrix-tree theorem and the Wiener Index*, Linear and Multilinear Algebra 25 (1989), 291–296.
- [24] B. Mohar, *Eigenvalues, Diameter, and Mean Distance in graphs*, Graphs and Combinatorics 7 (1991), 53–64.
- [25] I. Motoc and A. Balaban, *Topological indices: intercorrelation, physical meaning, correlational ability*, Revue Roumaine de Chimie 26 (1981), 593–600.
- [26] J. Plesnik, *On the sum of all distances in a graph or digraph*, J. Graph Theory 8 (1984), 1–21
- [27] O. Polansky, M. Randić, and H. Hosoya, *Transfer Matrix Approach to the Wiener Numbers of Catacondensed Benzenoids*, MATCH 24 (1989) 3–28.
- [28] M. Randić, *On Generalization of Wiener Index for Cyclic Structures*, Acta Chimica Slovenica, 49 (2002), 483–496.
- [29] D. H. Rouvray, *The modelling of chemical phenomena using topological indexes*, J. Comput. Chem. 8(1987), 470–480.
- [30] B. E. Sagan, Y.-N. Yeh, and P. Zhang, *The Wiener Polynomial of a Graph*, Int'l J. of Quant. Chem. 60 (1996) 959–969.
- [31] H. P. Schultz, *Topological Organic Chemistry, 1. Graph theory and topological indices of alkanes*, J. Chem. Info. Comput. Sci. 29 (1989) 227–228.
- [32] L. Šoltés, *Transmission in graphs: a bound and vertex removing*, Math. Slovaca 41 (1991), 11–16
- [33] N. Trinajstić, *Chemical Graph Theory*, Vol. 2, CRC Press, Boca Raton (1983),
- [34] H. Wiener, *Structural determination of paraffin boiling points*, J. A. Chem. Soc. 69 (1947), 17–20.
- [35] B.-Y. Yang, and Y.-N. Yeh, *Zigging and Zagging in Pentachains*, Adv. in Appl. Math. 16 (1995) 72–94.
- [36] B.-Y. Yang, and Y.-N. Yeh, *Chains of Motley Gems and their Wiener Indices*, in Proc. of First International Tainan-Moscow Algebra Workshop (Tainan, 1994), 329–349, de Gruyter (Berlin), 1996, Y. Fong *et al* eds.
- [37] B.-Y. Yang, and Y.-N. Yeh, *About Wiener Numbers and Polynomials*, in Proc. of Second International Tainan-Moscow Algebra Workshop (Tainan, 19978), 203–226, Springer (Hong Kong), 2000, Y. Fong *et al* eds.
- [38] B.-Y. Yang, and Y.-N. Yeh, *A Crowning Moment for Wiener Indices*, Stud. in Appl. Math. 112 (2004), 333–340.
- [39] B.-Y. Yang, and Y.-N. Yeh, *Wiener Polynomials of Some Chemically Interesting Graphs*, Int'l J. of Quant. Chem. 99 (2004), 80–91.
- [40] B. Zmazek, and J. Žerovnik, *Computing the weighted wiener and szeged number on weighted cactus graphs in linear time*, Croat. Chem. Acta 76(2)(2003), 137–143.