Acta Applicandae Mathematicae **72:** 247–294, 2002.

Wiener Index of Hexagonal Systems

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(Received: 5 December 2001)

Abstract. The Wiener index W is the sum of distances between all pairs of vertices of a (connected) graph. Hexagonal systems (HS's) are a special type of plane graphs in which all faces are bounded by hexagons. These provide a graph representation of benzenoid hydrocarbons and thus find applications in chemistry. The paper outlines the results known for W of the HS: method for computation of W, expressions relating W with the structure of the respective HS, results on HS's extremal w.r.t. W, and on integers that cannot be the W-values of HS's. A few open problems are mentioned. The chemical applications of the results presented are explained in detail.

Mathematics Subject Classifications (2000): 05-02, 05C12, 92-02, 92E10, 68R10.

Key words: Wiener index, hexagonal system, hexagonal chain, catacondensed hexagonal system, isometric subgraph, congruence relation, Hosoya polynomial, algorithm.

Introduction

THE WIENER INDEX

In this article, all graphs are finite, undirected, connected, without loops and multiple edges. The vertex and edge sets of a graph G are $V(G)$ and $E(G)$. The numbers of vertices and edges of G are denoted by $p = p_G$ and $q = q_G$, respectively.

Under *distance* $d_G(u, v)$ between vertices $u, v \in V(G)$ we mean the standard distance of the simple graph G, i.e., the number of edges on a shortest path connecting these vertices in G ([4]). The *distance of a vertex* $v \in V(G)$, $d_G(v)$, is the sum of distances between v and all other vertices of G.

The *Wiener index* is a graph invariant based on distances in a graph. It is denoted by $W(G)$ and defined as the sum of distances between all pairs of vertices in G:

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u, v) = \frac{1}{2} \sum_{v\in V(G)} d_G(v). \tag{1}$$

The name *Wiener index* or *Wiener number* for the quantity defined in Equation (1) is usual in chemical literature, since Harold Wiener [119], in 1947, seemed to be the first to consider it. Wiener himself used the name *path number*, but denoted his quantity by w. Wiener's original definition was slightly different – yet equivalent – to (1). The definition of the Wiener index in terms of distances between vertices of a graph, such as in Equation (1), was first given by Hosoya [75].

Starting from the middle of the 1970s, the Wiener index gained much popularity and, since then, new results related to it are constantly being reported. For a review, historical details and further bibliography on the chemical applications of the Wiener index see [69, 72, 97].

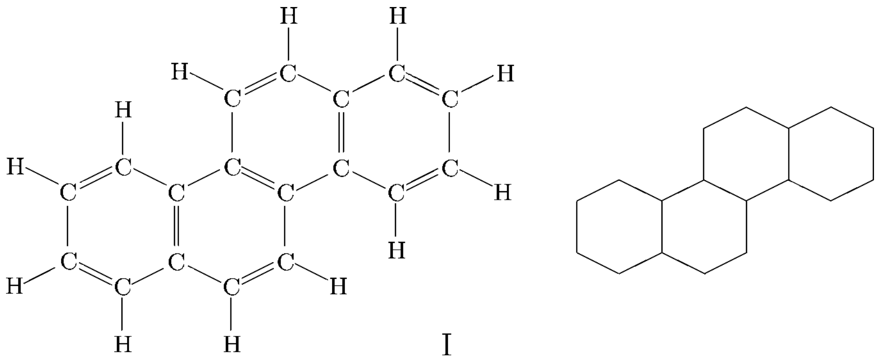
In the mathematical literature, W seems to have been first studied only in 1976 ([39]). For a long time, mathematicians were unaware of the (earlier) work on W done in chemistry (cf. the book [4]). Nevertheless, recent mathematical papers devoted to W give due credit to Wiener and name W after him. Other names for W found in the literature are *distance of a graph* ([39]) and *transmission* ([100]). Several mathematical papers deal with a closely related invariant – the *average distance*, defined as $\mu(G) = W(G)/\binom{p}{2}$, cf. [10].

Two groups of problems can be distinguished in the theory of the Wiener index: (a) how W depends on the structure of a graph and (b) how W can be efficiently calculated (including the so-called 'paper-and-pencil' methods). Finding simple conditions that provide the coincidence of the Wiener index for nonisomorphic graphs is of interest both in theoretical investigations and in applications. The greatest progress in solving the above problems was made for trees and hexagonal systems. Results on the Wiener index of trees were summarized in [34, 38] and in the recent review [30]. In the present paper, we outline the results achieved in the theory of the Wiener index of hexagonal systems.

CHEMICAL CONNECTIONS

From what has been said in the preceding section, it is clear that chemical problems have much influenced the development of the theory of the Wiener index. In fact, the Wiener index belongs to the molecular structure-descriptors, called *topological indices*, that are nowadays extensively used in theoretical chemistry for the design of so-called *quantitative structure-property relations* (QSPR) and *quantitative structure-activity relations* (QSAR), where under 'property' are meant the physico-chemical properties and under 'activity', the pharmacologic and biological activities of the respective chemical compounds. For details see the recent books [11, 12, 14, 117] and the references quoted therein.

The Wiener index found its first, simplest and most straightforward applications within modeling of the properties of acyclic molecules, so-called alkanes. This stimulated the elaboration of the theory of Wiener indices of trees (for details, see [30]).



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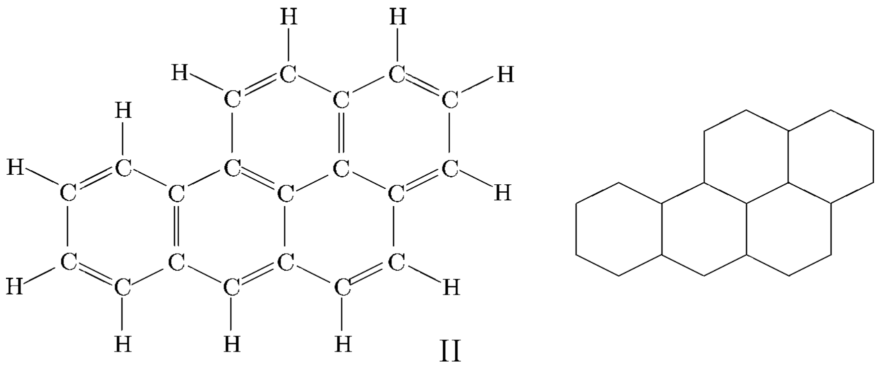

II

Figure 1. Two benzenoid hydrocarbons: chrysene (I) and benzo[a]pyrene (II) and the respective hexagonal systems; compound II is the carcinogenic constituent of tobacco smoke and other stuff.

However, the vast majority of molecules of interest in chemistry are cyclic. A plethora of types of cyclic molecules exist and, as a consequence, very few general mathematical results are known for their Wiener indices (or, more generally, for their topological indices). Mathematical research is of use only within classes of (molecular) graphs having some common and uniform structural features.

Fortunately, there is such a class of molecules: the *benzenoid hydrocarbons*. The carbon-atom skeleton of these hydrocarbons consists of mutually fused hexagons; two self-explanatory examples are depicted in Figure 1, together with the respective hexagonal systems. Benzenoid hydrocarbons possess intriguing (and somewhat mysterious) electronic properties and have been attracting the interest of theoretical chemists for well over 150 years. In addition, they are important raw materials of the chemical industry (used, for instance, for the production of dyes and plastics), but are also dangerous pollutants ([51, 120]). Around 1000 distinct benzenoid hydrocarbons are known nowadays, some of which consist of more than 100 hexagons. For recent progress in their detection, synthesis, and identification, see the reviews [74, 118].

After the hexagonal systems is defined in the subsequent section it will immediately become clear that the molecular graphs (or, more precisely, the graphs representing the carbon-atom skeleton), of benzenoid hydrocarbons are hexagonal systems. Because of this chemical connection (in addition to other reasons), the mathematical theory of hexagonal systems is nowadays being greatly expanded (see, for instance, [9, 43]). One direction of research along these lines is the study of the Wiener index of hexagonal systems. The main results achieved are collected in the present survey.

1. Hexagonal Systems and their Structure

1.1. HEXAGONAL SYSTEMS

In the existing (both mathematical and chemical) literature, there is considerable non-uniformity and inconsistency in the terminology pertaining to (what we call here) 'hexagonal systems'. In order to avoid any confusion, we first define our objects and their classification.

When consulting the respective literature, a neophyte in this areas may be amused and confused by the variety of names used for the species considered in this article. Among these, we mention (in alphabetical order) benzenoid graph, benzenoid system, fusene (perifusene, catafusene), hexagonal animal, hexagonal-cell configuration, hexagonal-cell system, hexagonal net, hexagonal polyomino, hexanimal, hex carpet, honeycomb system, lattice animal, polygon, polyhex, wall. It has already been explained in the Introduction why a considerable number of these names are of chemical origin.

It should be noted that in some papers (e.g., in [106]) under 'hexagonal system' is meant what here we refer to as 'simple hexagonal system'. In fact, the majority of published studies of hexagonal systems is restricted to simple hexagonal systems and this is often tacitly understood without being explicitly mentioned. Those hexagonal system which we describe here as 'jammed' are called 'geometrically nonplanar' or 'helicenic' in the earlier literature.

We proceed now with defining our own vocabulary.

A vertex v of a graph G is said to be a *cut-vertex* if the subgraph obtained by deleting v from G has more components than G.

In what follows, a six-membered cycle (a cycle embracing six vertices) will be referred to as a *hexagon*. Hexagonal systems are a special type of plane graphs, in which all interior regions (faces) are bounded by hexagons.

DEFINITION. A *hexagonal system* is a connected plane graph without cut-vertices in which all inner faces are hexagons (and all hexagons are faces), such that two hexagons are either disjoint or have exactly one common edge, and no three hexagons share a common edge. The sets of all hexagonal systems and of all hexagonal systems with h hexagons are denoted by HS and HS_h, respectively.

DEFINITION. A hexagonal system is said to be *simple* if it can be embedded into the regular hexagonal lattice in the plane without overlapping of its vertices. Hexagonal systems that are not simple are called *jammed*. The sets of all simple and jammed hexagonal systems are denoted by *sHS* and *jHS*, respectively. The sets of these species with h hexagons are sHS_h and jHS_h, respectively. Of course,

$$sHS \cap jHS = \emptyset, \qquad sHS_h \cup jHS_h = HS_h, \quad \text{and} \quad sHS \cup jHS = HS.$$

An alternative geometrical definition of simple hexagonal systems does not include the notion of the lattice ([106]). Namely, simple hexagonal systems are connected plane graphs with no cut-vertices in which every face is bounded by a regular hexagon of length 1.

An example of a simple hexagonal system (G_1) and a jammed hexagonal system (G_2) is depicted in Figure 2.

Hexagons sharing a common edge are said to be *adjacent*. Two hexagons of a hexagonal system may have either two common vertices (if they are adjacent) or none (if they are not adjacent). A vertex of a hexagonal system belongs to, at most, three hexagons. A vertex shared by three hexagons is called an *internal vertex* of the respective hexagonal system. The number of internal vertices is denoted by n_i.

DEFINITION. A hexagonal system is said to be *catacondensed* if it does not possess internal vertices ($n_i = 0$). A hexagonal system is said to be *pericondensed* if it possesses at least one internal vertex ($n_i > 0$). The sets of all catacondensed and pericondensed hexagonal systems are denoted by *CHS* and *PHS*, respectively. The sets of these species with h hexagons are CHS_h and PHS_h, respectively. Of course,

$$CHS \cap PHS = \emptyset, \qquad CHS_h \cup PHS_h = HS_h, \quad \text{and} \quad CHS \cup PHS = HS.$$

In Figure 2, G_1 and G_2 are catacondensed hexagonal systems; G_3 has two internal vertices and is therefore pericondensed.

By construction, the vertices of a hexagonal system are either of degree 2 or of degree 3. (The degree of a vertex u is denoted $\deg(u)$.) Every hexagonal system with h hexagons and n_i internal vertices has $p = 4h + 2 - n_i$ vertices and $q = 5h + 1 - n_i$ edges. The number of vertices of degree 2 and 3 is then $2h + 4 - n_i$ and $2h - 2$, respectively.

The difference between systems of the above two classes can be visually described by means of their characteristic graphs. The *characteristic* graph (or dualist, or inner dual) of a given hexagonal system consists of vertices corresponding to hexagons of the system; two vertices are adjacent if and only if the corresponding hexagons are adjacent.

Now, the characteristic graph of $G \in HS$ is a tree if and only if $G \in CHS$. Clearly, this tree has h vertices and none of its vertices has degree greater than 3. The characteristic graph of a pericondensed hexagonal system contains at least one

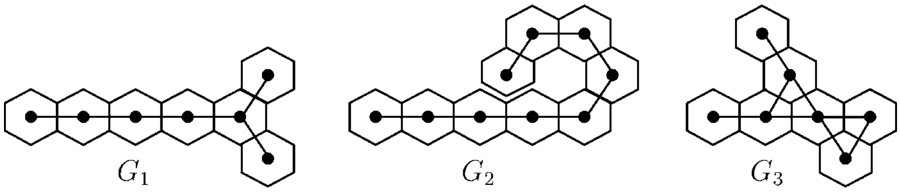

Figure 2. Simple hexagonal system G_1, jammed hexagonal system G_2, pericondensed hexagonal system G_3, and their characteristic graphs.

cycle (a triangle). Hexagonal systems and their characteristic graphs are also shown in Figure 2.

A hexagon r of a catacondensed hexagonal system has either one, two or three neighboring hexagons. If r has one neighboring hexagon, then it is said to be *terminal*, and if it has three neighboring hexagons, to be *branched*. Hexagons being adjacent to exactly two other hexagons are classified as angularly or linearly connected (mode A or L). A hexagon r adjacent to exactly two other hexagons possesses two vertices of degree 2. If these two vertices are adjacent, then r is *angularly connected*, for short we say that r is *of mode* A. If these two vertices are not adjacent, then r is *linearly connected*, and we say that r is *of mode* L.

DEFINITION. A catacondensed hexagonal system possessing at least one branched hexagon is said to be a *branched catacondensed hexagonal system*. A catacondensed hexagonal system without branched hexagons is called a *hexagonal chain*. The sets of all hexagonal chains and of all hexagonal chains with h hexagons are denoted by *HC* and HC_h, respectively.

Each of the above defined types of hexagonal systems can be either simple or jammed. Consequently, the sets *CHS*, CHS_h, *PHS*, PHS_h, *HC*, HC_h are partitioned into *sCHS*, $sCHS_h$, *sPHS*, $sPHS_h$, *sHC*, sHC_h and *jCHS*, $jCHS_h$, *jPHS*, $jPHS_h$, *jHC*, jHC_h, respectively.

In what follows, and where no confusion is possible, the descriptor ‘hexagonal’ will often be omitted. For instance, instead of ‘catacondensed hexagonal system’ and ‘zigzag hexagonal chain’ we shall say ‘catacondensed system’ and ‘zigzag chain’, respectively.

1.2. SEGMENTS OF CATACONDENSED HEXAGONAL SYSTEMS

Each branched and angularly connected hexagon in a catacondensed hexagonal system is said to be a ‘*kink*’, in contrast to the terminal and linearly connected hexagons. In the system G_4 shown in Figure 3 the kinks are marked by K.

The *linear chain* L_h with h hexagons is the catacondensed system without kinks. (Thus, for $h \geqslant 2$, L_h possesses two terminal and $h - 2$ L-mode hexagons.)

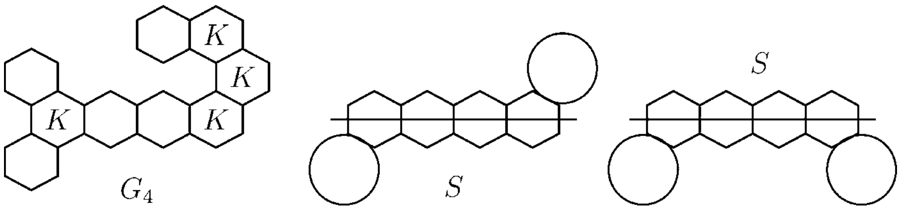

Figure 3. Kinks of a hexagonal system and types of segments.

A *segment* is a maximal linear chain in a catacondensed system, including the kinks and/or terminal hexagons at its end. A segment including a terminal hexagon is a *terminal segment*. The number of hexagons in a segment S is called its *length* and is denoted by $\ell(S)$. For any segment S of $G \in CHS_h$, $2 \leqslant \ell(S) \leqslant h$. We say that G consists of the set of segments $S_1, S_2, \ldots, S_n$ with lengths $\ell(S_i) = \ell_i$ for some $n \geqslant 1$. Since two neighboring segments have always one hexagon in common, the number of hexagons of $G \in CHS_h$ is equal to $h_G = \ell_1 + \ell_2 + \cdots + \ell_n - n + 1$.

For example, the hexagonal system G_4 of Figure 3 consists of one segment of length 4 and five segments of length 2.

For simple hexagonal chains or chain-like parts of other elements of *HS*, we distinguish two kinds of segments. Consider a nonterminal segment S with its two neighboring segments embedded into the regular hexagonal lattice in the plane and draw a line through the centers of the hexagons of S (see Figure 3). If the neighboring segments lie on different sides of the line, then S is called a *zigzag* segment. If these segments lie on the same side, then S is said to be a *nonzigzag* segment. It is convenient to consider that also the terminal segments are zigzag segments.

2. Hexagonal Systems Extremal with Respect to the Wiener Index

Several classes of hexagonal systems are considered in this section. For each of them, we specify its extremal element(s) with respect to W.

The *helix* H_h is a hexagonal chain whose all nonterminal segments are non-zigzag and have length 2 (see Figure 4). Note that $H_1 = L_1$ and $H_2 = L_2$.

2.1. HEXAGONAL CHAINS, HC_h

Inclusions: $HC_h \subset CHS_h$.

The extremal elements of this class are the linear chain L_h and the helix H_h (see Figure 4).

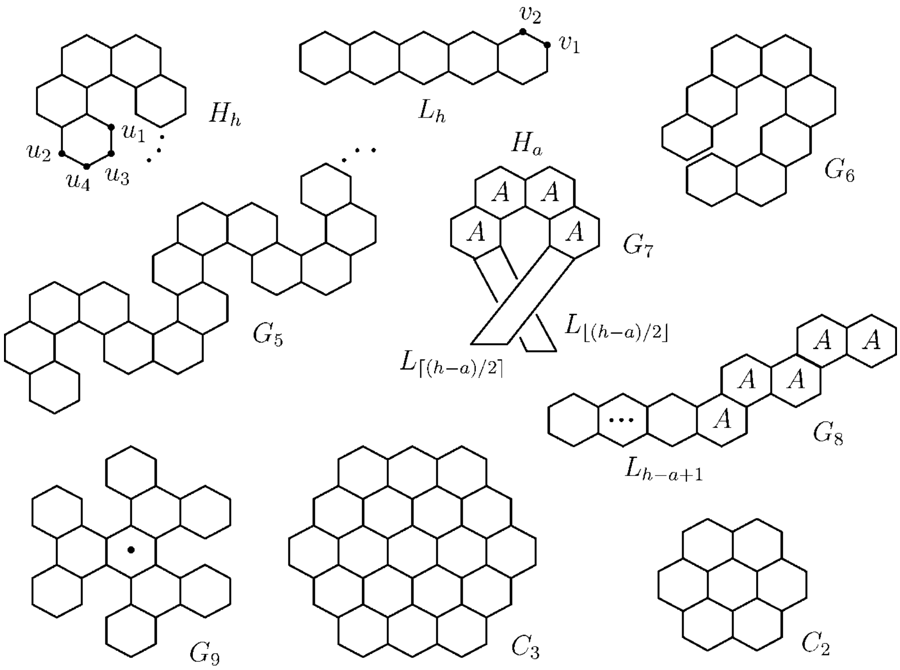

Figure 4. Some extremal hexagonal systems.

This pair of classes of graphs plays an important role in the theory of hexagonal systems (cf. [73]). Their Wiener indices are cubic polynomials in h and for any $G \in HC_h \setminus \{L_h, H_h\}$, $h \geqslant 4$ ([3, 41, 67]),

$$W(H_h) < W(G) < W(L_h),$$

where

$$W(L_h) = \tfrac{1}{3}(16h^3 + 36h^2 + 26h + 3),$$

and

$$W(H_h) = \tfrac{1}{3}(8h^3 + 72h^2 - 26h + 27).$$

Recall that for $h \leqslant 3$, $HC_h \setminus \{L_h, H_h\} = \emptyset$.

Distances of vertices in the terminal hexagons of these systems are also extremal. For vertices v_1, v_2 of the linear chain L_h and u_1, u_2, u_3, u_4 of the helix H_h (see Figure 4), one has ([17])

$$d(v_1) = 4h^2 + 4h + 1, \qquad d(v_2) = 4h^2 + 5$$

and

$$d(u_1) = 2h^2 + 6h + 1, \qquad d(u_2) = 2h^2 + 10h - 3,$$

$$d(u_3) = 2h^2 + 10h - 7, \qquad d(u_4) = 2h^2 + 14h - 11.$$

2.1.1. *Simple Hexagonal Chains, sHC_h*

Inclusions: $sHC_h = HC_h \cap sHS_h$.

The maximum and minimum Wiener indices are realized on the linear chain L_h and the serpent S_h, respectively. The structure of the *serpent* should be clear from the example G_5 depicted in Figure 4 ([19]). Note that $S_h = H_h$ for $1 \leqslant h \leqslant 5$. For these graphs

$$W(S_h) = \tfrac{1}{9}(32h^3 + 168h^2 + \phi(h)),$$

where

$$\phi(h) = \begin{cases} -6h + 81, & \text{if } h = 3m, m = 1, 2, 3, \ldots, \\ -6h + 49, & \text{if } h = 3m + 1, m = 0, 1, 2, \ldots, \\ -6h + 161, & \text{if } h = 3m + 2, m = 0, 1, 2, \ldots. \end{cases}$$

2.1.2. *Jammed Hexagonal Chains, jHC_h*

Inclusions: $jHC_h = HC_h \setminus sHC_h$.

Elements of jHC_h exist for $h \geqslant 6$. The extremal elements are the helix H_h and the *hook* (cf. G_2 in Figure 2) for which

$$W(G_2) = \tfrac{1}{3}(16h^3 + 36h^2 - 358h + 1587) + C,$$

where $C = 8$ if $h = 8$ and $C = 0$ otherwise [19]. Exceptionally, for $h = 8$ the jammed chain with maximum Wiener index is G_6, depicted in Figure 4; $W(G_6) = 3081$ while the Wiener index of the hook is equal to 3073.

2.1.3. *Zigzag Hexagonal Chains, ZHC_h*

Inclusions: $ZHC_h \subset sHC_h$.

A graph of this class has zigzag segments only. By definition of the zigzag segment, the linear chain L_h belongs to ZHC_h. If all segments of a system G are of length 2, then this unique system has minimum Wiener index among all elements of ZHC_h. Its W-value was determined in [3]:

$$W(G) = \tfrac{1}{3}(16h^3 + 24h^2 + 62h - 21).$$

2.1.4. *Fibonacenes, FHC_h*

Inclusions: $FHC_h \subset HC_h$.

A fibonacene is a hexagonal chain in which all hexagons, apart from the two terminal ones, are angularly connected, for instance, the graphs H_h and G_5 of Figure 4. The name of these chains comes from the fact that the number of perfect matchings of any $G \in FHC_h$ is equal to the $(h + 1)$th Fibonacci number. (This result is of some significance in chemical applications, see [51].)

The helix H_h, $h \geqslant 3$, has the minimal Wiener index in this class, whereas the element G of FHC_h with maximum W-value coincides with the element of ZHC_h with the minimum W-value. This fact and the expressions for the Wiener index of the next two subsections easily follow from the results of Section 5.

2.1.5. *Chains with Given Number of A-Mode Hexagons, $HCA_{h,a}$*

Inclusions: $HCA_{h,a} \subset HC_h$.

A hexagonal system from $HCA_{h,a}$ has exactly a hexagons of mode A, $h-a-2$ hexagons of mode L, and two terminal hexagons. This class contains some of the above-described classes for the corresponding values of a. For example, $FHC_h = HCA_{h,h-2}$. A number of elements of $HCA_{h,a}$ have the maximal Wiener index (this fact is explained in Section 5). One such system with $a = 5$ is G_8, shown in Figure 4, and

$$W(G_8) = \tfrac{1}{3}(16h^3 + 36h^2 - 2h(12a - 13) - 4a^3 + 12a^2 + 40a + 3).$$

The graph G_7 with minimal Wiener index consists of the helix H_a and two equal linear chains $L_{\lfloor (h-a)/2 \rfloor}$ and $L_{\lceil (h-a)/2 \rceil}$ attached to the terminal hexagons of H_a as shown in Figure 4 for $a = 4$ (G_7 coincides with H_h for $h \leqslant 6$). This system is unique and

$$\begin{aligned} W(G_7) \;=\; & \tfrac{1}{3}(16h^3 - 6h^2(2a - 7) + 2h(18a + 1) \;+ \\ & + 4a^3 - 6a^2 - 28a + 27) + \phi(h, a), \end{aligned}$$

where $\phi(h, a) = 2(2a - 1)$ if $h - a$ is even and $\phi(h, a) = 0$, otherwise.

2.1.6. *Hexagonal Chains with Equal Segments, EHC_h*

Inclusions: $FHC_h \subset EHC_h \subset HC_h$.

The number of segments n and their length ℓ define the number of hexagons in these chains: $h = n(\ell - 1) + 1$. A condition for the existence of such systems is that the number of segments $n = (h - 1)/(\ell - 1)$ must be an integer. The number of hexagons of mode A is equal to $a = n - 1$. The structure of the unique extremal systems is obvious. The system G' with minimal Wiener index is the chain in which all segments (except the two terminal) are nonzigzag. The system G'' with maximal W has all segments in zigzag arrangement. Further,

$$\begin{aligned} W(G') \;=\; & \frac{1}{3(\ell - 1)}(8h^3(2\ell - 3) + 24h^2(2\ell - 1) + 2h(2\ell^2 - 5\ell + 15) \;+ \\ & + 4\ell^2 + 7\ell - 3), \\ W(G'') = \; & \tfrac{1}{3}\big(16h^3 + 24h^2 + 2h(6\ell + 19) - 12\ell + 3\big). \end{aligned}$$

2.2. CATACONDENSED HEXAGONAL SYSTEMS, CHS_h

The linear chain L_h has the maximum Wiener index. For branched catacondensed systems, the extremal graph G_1 is the one depicted in Figure 2. We have ([26]):

$$W(G_1) = \frac{1}{3}(16h^3 + 36h^2 - 118h + 411).$$

The system having the minimum Wiener index is clear (see graph G_9 in Figure 4 for $h = 10$), but an analytic expression for its W-value is not known. Every nonterminal hexagon (maybe except one) of such a system must be branched.

2.2.1. *Simple Catacondensed Hexagonal Systems, sCHS$_h$*

The linear chain L_h has the maximum Wiener index. The system with minimum W has the same structure as for catacondensed systems up to $h = 10$ hexagons. An analytic expression for W of the system with the minimal W is not known.

2.3. PERICONDENSED HEXAGONAL SYSTEMS, *PHS*

2.3.1. *Simple Pericondensed Hexagonal Systems, sPHS*

Since the number of hexagons and the number of vertices do not directly depend, it is worth considering two subclasses of *sPHS*.

(a) Simple pericondensed systems with a fixed number h of hexagons, *sPHS*$_h$. The structure of a system with maximal W depends on the number n_i of internal vertices. If $n_i = 1$, then the respective system (denoted by G'), contains L_{h-1} and its hth hexagon is adjacent to the first and second hexagons of L_{h-1}. If $n_i = 2$, then G'' contains L_{h-2} and every terminal hexagon of L_{h-2} has an internal vertex in G''. For these cases ([3]),

$$W(G') = \frac{1}{3}(16h^3 + 24h^2 - 70h + 192)$$

and

$$W(G'') = \frac{1}{3}(16h^3 + 12h^2 - 160h + 438).$$

The hexagonal system C_2 shown in Figure 4 is referred to as the *coronene* (a name borrowed from chemistry). Circumscribing C_2 by hexagons, we obtain the *circumcoronene* (see C_3 in Figure 4). The structure of the further members $C_4, C_5, \ldots$ of the circumcoronene series is evident. For basic properties of circumcoronenes see [53].

The circumcoronene-like systems have minimal W-values. These systems can be obtained from circumcoronenes C_k by deleting their peripheral hexagons. The number of hexagons of C_k is $h = 3k^2 - 3k + 1$ and [61, 108]

$$W(C_k) = \frac{1}{5}(164k^5 - 30k^3 + k). \tag{2}$$

(b) Simple pericondensed systems with a fixed number p of vertices *sPHS*^{p}. Such classes are considered in chemical applications. Circumcoronene C_k has $p = 6k^2$ vertices and it has minimum Wiener index for systems with this order. The structure of a system with maximal W also depends on the number of internal vertices. Graphs of this class may have a different number of hexagons. For two arbitrary systems G_1 and G_2 of PHS^p, the relation $4(h_1 - h_2) = n_{i1} - n_{i2}$ holds, i.e., the numbers of their internal vertices are congruent modulo 4. Thus, the above system G' with h' hexagons and one internal vertex has maximum W among all simple pericondensed systems G with $h = h' + (n_i - 1)/4$ hexagons and n_i internal vertices.

2.3.2. *Pericondensed Hexagonal Systems, PHS*

The extremal systems are the same as for simple pericondensed systems.

3. Algorithms for Computing the Wiener Index

Let G be a graph. To compute the Wiener index of a graph, it clearly suffices to compute the distances between all pairs of vertices of G. Floyd and Warshall's algorithm and the BFS algorithm are two standard algorithms for this task that can be found in (almost) any textbook on (graph) algorithms. They run in $\mathcal{O}(p^3)$ and $\mathcal{O}(pq)$ time, respectively. Since in hexagonal systems $q = \mathcal{O}(p)$ we can thus compute the Wiener index of a hexagonal system in $\mathcal{O}(p^2)$ time (cf. [96]). In this section we show that the complexity of computing the Wiener index of a hexagonal system can be reduced to $\mathcal{O}(p)$. Moreover, one can even develop a sublinear time algorithm for simple hexagonal systems. Before presenting these algorithms, some preparation from the metric graph theory is needed.

3.1. ISOMETRIC EMBEDDINGS OF HEXAGONAL SYSTEMS

Let G be a connected graph. Then its subgraph H is said to be *isometric* if, for any pair of vertices u, v of H, we have $d_G(u, v) = d_H(u, v)$. For instance, any hexagon of a hexagonal system is its isometric subgraph.

The *n-cube* Q_n is the graph constructed as follows. The vertex set of Q_n consists of all strings of length n over {0, 1} and two such strings are adjacent if they differ in exactly one position. A graph is called a *hypercube* if it is isomorphic to some n-cube. Clearly, Q_n has 2^n vertices, is n-regular, and has diameter n. The starting point for investigations in this direction is the following result:

THEOREM 3.1. *Any hexagonal system is an isometric subgraph of a hypercube.*

Theorem 3.1 is given in [85] for simple hexagonal systems but holds for the general case as well. We now briefly describe how one can construct such an embedding.

Let G be a hexagonal system. We partition the edge set of G into edge-subsets $E_1, E_2, \ldots, E_k$ as follows. Let e be an edge of G and f an opposite edge of a hexagon to which e belongs. Then both e and f belong to the same class E_i. Inductively filling the edge-subsets in this way, we end up with a partition of the edge set of G. For instance, for the graph C_2 of Figure 4, the corresponding partition consists of 9 edge-subsets while for the graph G_6 of the same figure, $k = 17$. Consider the graphs $G_i = G \setminus E_i$ for $i = 1, 2, \ldots, k$. They consist of two connected components, say G_i^0 and G_i^1. We now assign a string $s(u)$ of length k to a vertex u of G as follows. Set the ith digit of $s(u)$ to 0 if $u \in G_i^0$ and to 1 if $u \in G_i^1$. In this way, to every vertex u of G we have assigned a vertex $s(u)$ of Q_k. Now it can be shown that in this way G is represented as an isometric subgraph of Q_k. We will use this embedding later in this section and also in Section 5 where it will be applied to obtain formulas for classes of hexagonal systems.

We next describe another isometric embedding of a hexagonal system that is essential for rapid computation of the Wiener index. For this purpose, the following concept is needed.

The *Cartesian product* $G \square H$ of graphs G and H is the graph with vertex set $V(G) \times V(H)$ and $((a, x), (b, y)) \in E(G \square H)$ whenever $(a, b) \in E(G)$ and $x = y$, or $a = b$ and $(x, y) \in E(H)$. The Cartesian product is commutative and associative. Hence, we may write $G = G_1 \square G_2 \square \cdots \square G_k$ for the Cartesian product of graphs $G_1, G_2, \ldots, G_k$. In this case, the vertex set of G is $V(G_1) \times V(G_2) \times \cdots \times V(G_k)$ and two vertices $(u_1, u_2, \ldots, u_k)$ and $(v_1, v_2, \ldots, v_k)$ are adjacent if they differ in exactly one position, say in ith, for which (u_i, v_i) is an edge of G_i. Note that the n-cube Q_n is just the Cartesian product of n copies of the complete graph on two vertices K_2. For more information on the Cartesian product of graphs and isometric subgraphs, see the book [79].

Let G be a hexagonal system and let the edge set of G be partitioned into edge-subsets $E_1, E_2, \ldots, E_k$ as described above. We combine some of these edge-subsets in order to obtain three edge-subsets F_1, F_2, F_3 as follows. Consider a hexagon $u_1u_2u_3u_4u_5u_6u_1$ of G and let it be adjacent to a hexagon $u_1u_2u_7u_8u_9u_{10}u_1$ (via the edge (u_1, u_2)). Suppose that the edge (u_3, u_4) belongs to E_i (as well as it does the edge (u_1, u_6)) and that the edge (u_2, u_7) belongs to E_j (as well as it does the edge (u_9, u_{10})). Then combine $E_i \cup E_j$ to the same F_ℓ. Inductively completing this construction, we end up with a partition of the edge set of G into three edge-subsets F_1, F_2, F_3. Let $G_i = G \setminus F_i$, $i = 1, 2, 3$, and let T_i be the graph whose vertices are connected components of G_i, two vertices of T_i being adjacent if there is an edge in G between the corresponding components of G_i. It turns out that T_i, $i = 1, 2, 3$, is a tree. This construction is illustrated in Figure 5.

Define a mapping $\alpha\colon G \to T_1 \square T_2 \square T_3$ as follows. For a vertex v of G set $\alpha(v) = (v_1, v_2, v_3)$, where v_i is the vertex of T_i corresponding to v. Now we have [6]:

THEOREM 3.2. *Let G be a hexagonal system. Then $\alpha(G)$ is an isometric subgraph of $T_1 \square T_2 \square T_3$.*

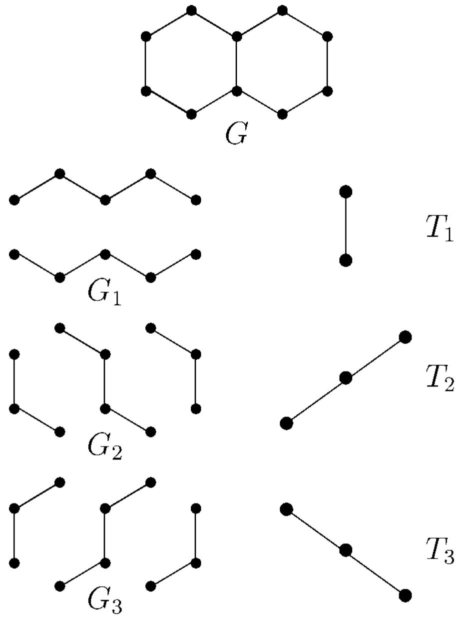

Figure 5. Hexagonal system G, graphs $G_i = G \setminus F_i$, and trees T_i, $i = 1, 2, 3$.

3.2. LINEAR AND SUBLINEAR ALGORITHM

Theorem 3.2 is the starting point for a linear algorithm for computing the Wiener index of hexagonal systems. We first observe ([6]) that the trees T_i and the corresponding labels of the vertices of a hexagonal system G can be computed in $\mathcal{O}(p)$ time.

We need yet another concept. A *weighted graph* (G, w) is a graph G together with a *weight function* $w\colon V(G) \to \mathbb{N}^+$. The Wiener index $W(G, w)$ of a weighted graph (G, w) is defined as [84]:

$$W(G, w) = \sum_{\{u,v\} \subseteq V(G)} w(u)w(v)d_G(u, v).$$

Note that if all the weights are 1, then $W(G, w) = W(G)$.

Let G be a hexagonal system, and T_1, T_2, T_3 the trees as in Theorem 3.2. For a vertex u of a tree T_i let the weight $w_i(u)$ be the number of vertices x of G, whose ith position in the label $\alpha(x)$ is equal to u. An example is given in Figure 6.

The second step for our algorithm is ([7]):

THEOREM 3.3. *Let G be a hexagonal system, and* (T_1, w_1), (T_2, w_2), *and* (T_3, w_3) *the corresponding weighted trees. Then*

$$W(G) = W(T_1, w_1) + W(T_2, w_2) + W(T_3, w_3).$$

By Theorem 3.3, a linear algorithm for computing $W(G)$ will be provided by a linear algorithm for computing the Wiener index of a weighted tree. This task was done implicitly in [96] and explicitly in [7]. We thus get:

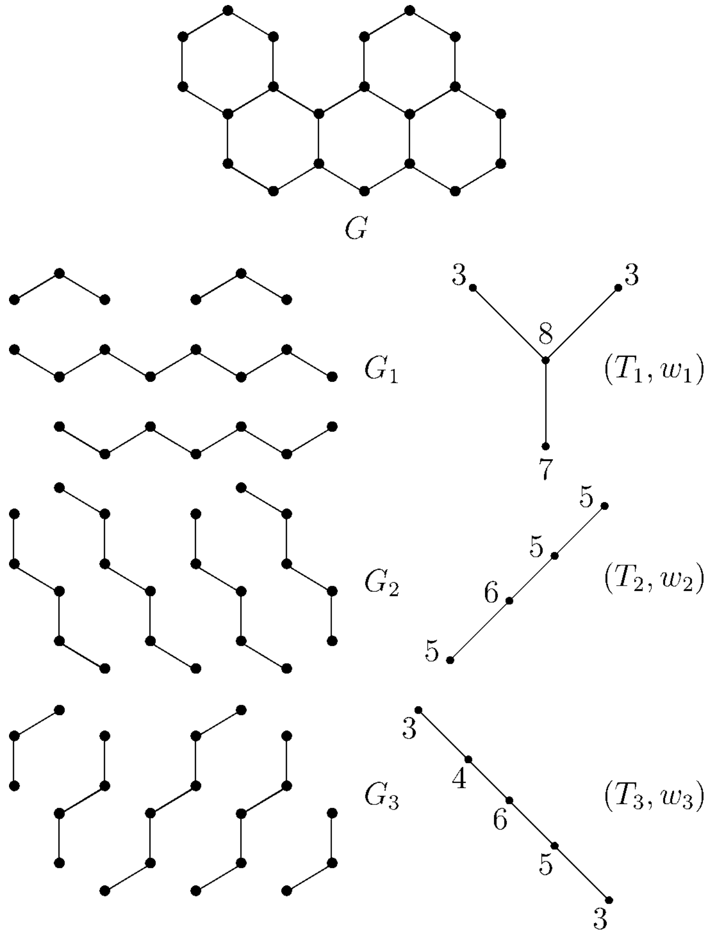

Figure 6. Hexagonal system G and the corresponding weighted trees (T_i, w_i).

THEOREM 3.4. *The Wiener index of a hexagonal system on p vertices can be computed in $\mathcal{O}(p)$ time.*

For the case of simple hexagonal systems, the Wiener index can be computed even faster. Consider a simple hexagonal system G embedded into the regular hexagonal lattice in the plane. Then G is formed by the vertices and edges of the lattice lying on a bounding circuit Z and in the interior of the region bounded by Z. Thus, G is completely determined by Z. We are going to briefly describe how $W(G)$ can be computed in $\mathcal{O}(|Z|)$ time (for details see [8]).

The main idea is that we can construct the weighted trees (T_1, π_1), (T_2, π_2), and (T_3, π_3) without an explicit definition of the facial structure of G. Let $\mathcal{D}$ denote the region of the plane bounded by Z. The algorithm is based on the Chazelle algorithm [5] for computing all vertex-edge visible pairs of edges of a simple polygon with n vertices. Applying the algorithm of Chazelle we find the subdivisions $\mathcal{D}_1$,

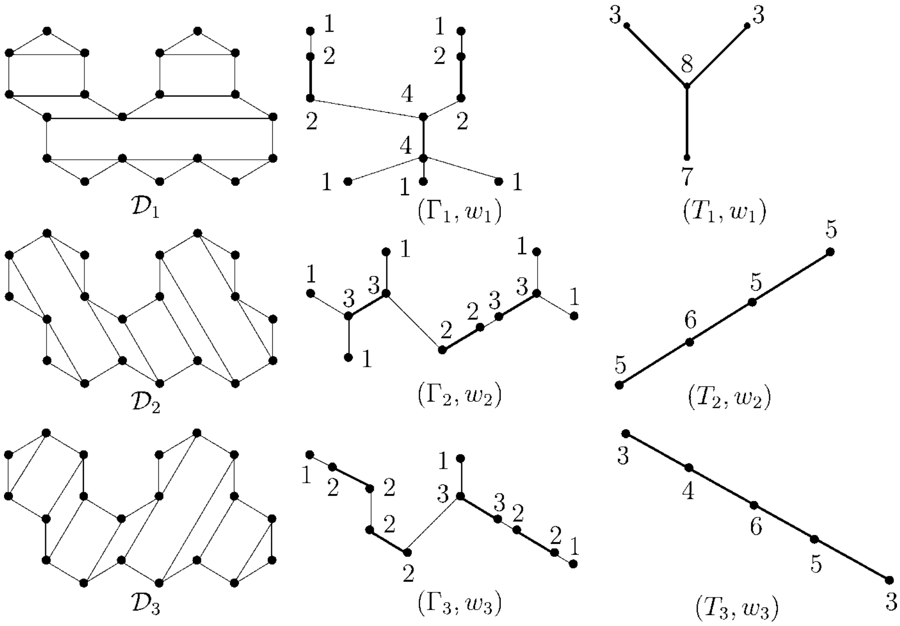

Figure 7. The subdivisions $\mathcal{D}_1$, $\mathcal{D}_2$, and $\mathcal{D}_3$, weighted trees (Γ_i, w_i), and weighted trees (T_i, w_i), $i = 1, 2, 3$.

$\mathcal{D}_2$, and $\mathcal{D}_3$ of the region $\mathcal{D}$ into strips; see Figure 7 for an illustration (some of strips can represent triangles).

Let $\mathcal{C}_i$ be the set of cuts participating in the subdivision $\mathcal{D}_i$. Define a new graph Γ_i whose vertices are the cuts of $\mathcal{C}_i$ (including the degenerated cuts consisting of single points) and two vertices of Γ_i are adjacent if they belong to a common strip of $\mathcal{D}_i$. The width of strips of $\mathcal{D}_i$ takes only two values, 1 and $1/2$. An edge of Γ_i is called *thick* if it is defined by a strip of width 1 and *thin* otherwise (cf. Figure 7 again). Every cut of $\mathcal{C}_i$ is incident in Γ_i to exactly one thick edge, all remaining vertices of $\mathcal{C}_i$ being incident only to thin edges. If we remove the thick edges of Γ_i, we will get the connected subgraphs of Γ_i spanned by thin edges (we will call them thin components). Every thin component of Γ_i has the same vertices of G as some connected component of the graph G_i. Hence, if we contract all thin edges of $\mathcal{C}_i$, we obtain the tree T_i.

4. Wiener Index of Growing Hexagonal Systems

By growth of a hexagonal system we mean a process of sequential increasing of the number of its hexagons. This may lead to increasing segment lengths or a number of segments. In this section several operations of this kind will be considered.

4.1. WIENER INDEX UNDER SUBGRAPH ATTACHMENT

Any hexagonal system can be regarded as being constructed by a recursive procedure of joining a hexagon to the previously constructed system. Thus, beginning from one hexagon, it is possible to obtain all elements of *HS*. For catacondensed systems this operation is quite simple ([67]):

THEOREM 4.1. *Let $G \in HS_h$ and $e = (v, u) \in E(G)$. If the system $G_1 \in HS_{h+1}$ is constructed from the G by identifying the edge e with an edge of a hexagon, then*

$$W(G_1) = W(G) + 2[d_G(u) + d_G(v)] + 6p_G + 10. \tag{3}$$

Many results in the theory of the Wiener index of hexagonal systems were derived by making use of Equation (3). Among them, we mention the basic congruence relation between W-values of catacondensed systems and numerous explicit expressions for the Wiener index of specific series of hexagonal systems [3, 41, 42, 58, 59, 65, 67, 77, 78, 86, 103, 109–113].

COROLLARY 4.1.1 *If $G \in CHS_h$, then*

$$W(G_1) = W(G) + 2[d_G(u) + d_G(v)] + 2(12h + 11).$$

If a hexagon joins with a terminal hexagon of G and v is adjacent with a vertex of degree 3, then

$$W(G_1) = W(G) + 4d_G(v) + 2(16h + 7).$$

If an element of *HS* is a result of joining via an edge of two other systems with smaller number of hexagons (see G_1 in Figure 8), then the Wiener index of the new system can be expressed through W of the initial systems and the distances of vertices incident to the identified edges [101].

THEOREM 4.2. *Let G_1, G_2 be arbitrary hexagonal systems and $e_1 = (v_1, u_1) \in E(G_1)$, $e_2 = (v_2, u_2) \in E(G_2)$. If the system G is constructed from G_1 and G_2 by identifying the edges e_1 and e_2 so that the vertex v_1 is identified with the vertex v_2, then*

$$\begin{aligned} W(G) \;=\; & W(G_1) + W(G_2) + \tfrac{1}{2}\{(p_{G_2} - 2)[d_{G_1}(v_1) + d_{G_1}(u_1)] + \\ & + (p_{G_1} - 2)[d_{G_2}(v_2) + d_{G_2}(u_2)] - [d_{G_1}(v_1) - d_{G_1}(u_1)] \times \\ & \times [d_{G_2}(v_2) - d_{G_2}(u_2)] - p_{G_1}p_{G_2}\} + 1. \end{aligned} \tag{4}$$

For an edge $e = (v, u)$, denote by $n_v(e)$ the number of vertices of the graph considered lying closer to v than to u, and by $n_u(e)$ the number of vertices lying closer to u than to v. For catacondensed systems, it is useful to apply Equation (4) written in the following form [16]:

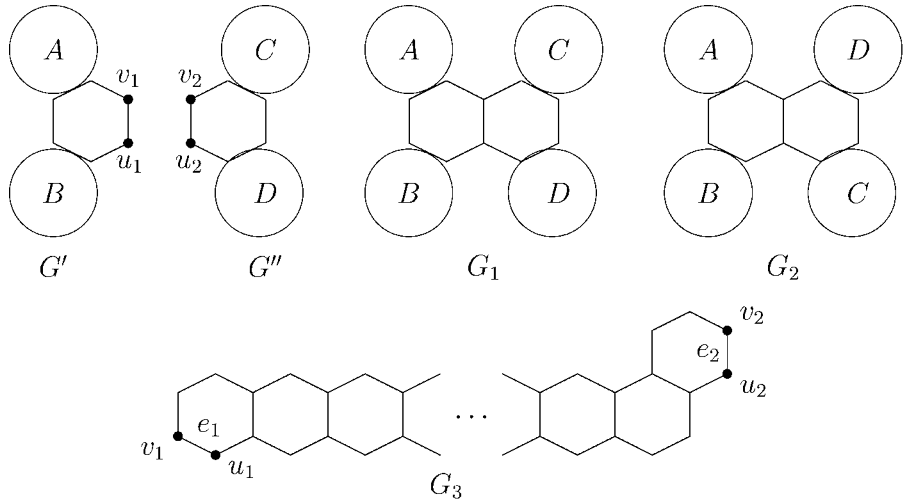

Figure 8. Attachment of hexagonal systems.

COROLLARY 4.2.1. *Let $G_1 \in CHS_{h_1}$, $G_2 \in CHS_{h_2}$ and $e_1 = (v_1, u_1) \in E(G_1)$, $e_2 = (v_2, u_2) \in E(G_2)$. If a hexagonal system G is obtained from G_1 and G_2 by identifying the edges e_1 and e_2 (v_1 is identified with v_2), then*

$$\begin{aligned} W(G) \;=\; & W(G_1) + W(G_2) + 4h_2 d_{G_1}(v_1) + 4h_1 d_{G_2}(v_2) + \\ & + 2[n_{u_1}(e_1) + n_{u_2}(e_2) - n_{u_1}(e_1) n_{u_2}(e_2)] - \\ & - 4(h_1 + h_2 + 1) + 1. \end{aligned} \tag{5}$$

Suppose that G_1 and G_2 are constructed from the same pair of hexagonal systems G' and G'' by identifying $e_1 = (v_1, u_1) \in E(G')$ with $e_2 = (v_2, u_2) \in E(G'')$. Let the vertex v_1 be identified with v_2 in G_1, while in G_2 the vertex v_1 is identified with u_2 (see Figure 8). Then the changes of the Wiener index can be presented in a simple way.

COROLLARY 4.2.2. *For the above described systems G_1 and G_2,*

$$W(G_1) - W(G_2) = [n_{v_1}(e_1) - n_{u_1}(e_1)][(n_{v_2}(e_2) - n_{u_2}(e_2)].$$

It follows that $W(G_1) = W(G_2)$ if and only if $h_A = h_B$ or $h_C = h_D$. The smallest example of such nonisomorphic systems obviously has seven hexagons. The change of W under other similar transformations is described in [3, 15, 16, 49, 50, 57, 101, 102].

In order to construct a catacondensed system, one can recursively join linear chains of different sizes instead of hexagons. Two edges (vertices) are called *equivalent* if there exists an automorphism that moves one edge (vertex) into other.

COROLLARY 4.2.3. *Let $G \in CHS_h$ and $e = (v, u) \in E(G)$ be an edge of a terminal hexagon. Let the hexagonal system G_1 be constructed by identifying the edge e and a terminal edge of the linear chain L_k. If the edge of L_k has equivalent incident vertices of degree* 2*, then*

$$W(G_1) = W(G) + W(L_k) + 4kd_G(v) - 4kn_u(e) + 16hk(k+1) - 1$$

(*the vertices v and u can be interchanged*). *If the edge e has one vertex of degree* 3 (*say, the vertex v*)*, then*

$$W(G_1) = W(G) + W(L_k) + 4kd_G(v) + 16hk(k+1) - 12k - 1.$$

As an illustration, consider the following problem: given a hexagonal system G, does there exist a pair of hexagonal systems with the same W that contain G as subgraphs? Applying formula (5) to the graph G_3 depicted in Figure 8 and to G, one can conclude that such a pair exists for every $h \geqslant h_G + 4$. Indeed, G_3 has equal vertex distances of nonequivalent edges e_1 and e_2 for all $h_{G_3} \geqslant 4$. Namely,

$$d(v_1) = d(v_2) = 4h^2 + 4h + 1,$$

$$d(u_1) = d(u_2) = 4h^2 + 5$$

and

$$n_{u_1}(e_1) = n_{u_2}(e_2) = p_{G_3} - 3.$$

Any edge of a terminal hexagon of G can be chosen for identifying.

4.2. KINK TRANSFORMATIONS OF HEXAGONAL SYSTEMS

Consider two graph operations of a catacondensed system G that consist in decomposing a terminal segment of G into new segments S_1 and S_2 as shown in Figure 9. In other words, a terminal part of S is displaced from its initial location in G_1 to another one making new kinks in the resulting graph G_2. Here A and B stand for arbitrary fragments; in particular, they may be absent. An inverse operation fuses the segments S_1 and S_2 into the terminal segment S (the lower arrows in Figure 9). These operations are called *kink transformations* [25].

THEOREM 4.3. *Let G be arbitrary element of CHS_h. Then G can always be obtained from the linear chain L_h by a sequence of kink transformations.*

Starting from the linear chain, two different systems G_1 and G_2 can be constructed. Then, making use of inverse kink transformation, it is always possible to realize the following transformations: $G_1 \to L_h \to G_2$.

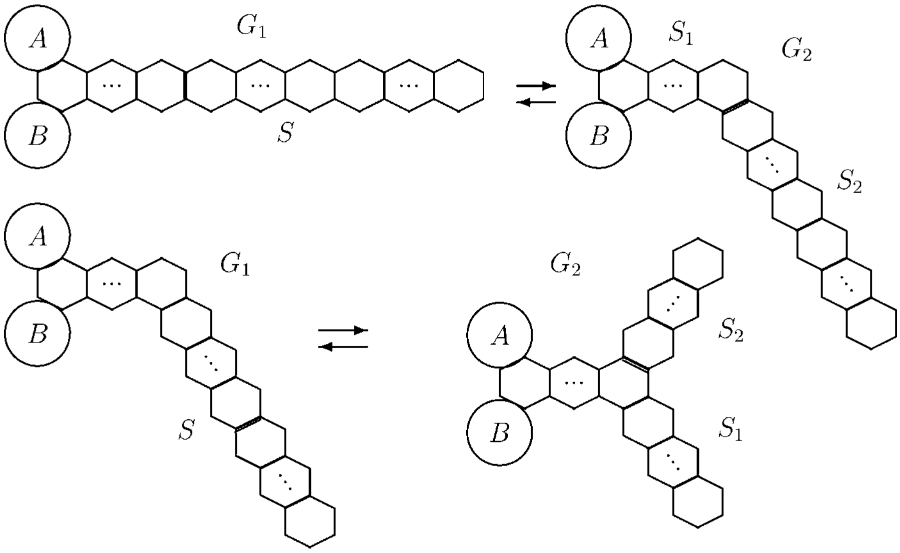

Figure 9. Kink transformations of hexagonal systems.

COROLLARY 4.3.1 *Let G_1 and G_2 be arbitrary elements of CHS_h. Then G_2 can always be obtained from G_1 by a sequence of kink transformations.*

Using Corollary 4.2.1, the change of the Wiener index can be expressed through simple structural parameters of graphs under these operations ([25]). Let $\ell_1 = \ell(S_1)$ and $\ell_2 = \ell(S_2)$.

THEOREM 4.4. *For the first kink transformation shown in Figure* 9,

$$W(G_1) - W(G_2) = 16(\ell_2 - 1)h_B + 8(\ell_1 - 1)(\ell_2 - 1).$$

For the second kink transformation shown in Figure 9

$$\begin{aligned} W(G_1) - W(G_2) &= 16(\ell_2 - 1)[2(\ell_1 - 1)(h_G - \ell_1) + h_A - h_B] + \\ &\quad + 8(\ell_1 - 1)(\ell_2 - 1). \end{aligned}$$

Let G and G' be arbitrary elements of CHS_h. By Corollary 4.3.1, G' may be obtained from G by a sequence of kink transformations:

$$G = G_1 \to G_2 \to \cdots \to L_h \to \cdots \to G_{m-1} \to G_m = G'.$$

Therefore,

$$W(G') - W(G) = \sum_{i=2}^{m} [W(G_i) - W(G_{i-1})].$$

As a rule, the analysis of the difference $W(G_i) - W(G_{i-1})$ for neighboring systems in the sequence is a simpler problem than the evaluation of $W(G') - W(G)$

at once. Using this approach various results described in the next sections were obtained [25–29].

4.3. RANDOM GROWTH OF HEXAGONAL CHAINS

If HC_h^* is the set of some (not necessarily all) hexagonal chains with h hexagons, then the average value of the Wiener index (with respect to HC_h^*) is

$$W_{\text{avr}}(HC_h^*) = \frac{1}{|HC_h^*|} \sum_{G \in HC_h^*} W(G).$$

A random hexagonal chain, R_h with h hexagons, $h > 2$, is a hexagonal chain obtained by stepwise addition of terminal hexagons. At each step $k = 2, 3, \dots, h$, a random selection is made from one of the three possible constructions (see Figure 10):

$R_{k-1} \to R_k^1$, with probability p_1,
$R_{k-1} \to R_k^2$, with probability p_2,
$R_{k-1} \to R_k^3$, with probability $q = 1 - p_1 - p_2$.

It is assumed that the probabilities p_1 and p_2 are constants, independent of the step k.

Random hexagonal chains offer a good model for a class of conjugated polymers (large benzenoid hydrocarbons in particular) ([90]).

The above described construction of the random chain R_h was put forward by Gutman, Kennedy and Quintas [58]. In what follows we refer to it as the GKQ-algorithm. The quantity $W(R_h)$ is a random variable. If R_h is constructed by means of the GKQ-algorithm, then the expected value W_h of $W(R_h)$ depends only on p_1, p_2 and h. The following result has been obtained for W_h [58]:

THEOREM 4.5. *Let a random hexagonal chain R_h be obtained by means of the GKQ-algorithm. Then $W_1 = 27$, $W_2 = 109$, $W_3 = 271 + 8q$ and for $h \geqslant 4$,*

$$\begin{aligned} W_h \ = \ & 4h^3 + 16h^2 + 6h + 1 + \tfrac{4}{3}q(h^3 - 3h^2 + 2h) - \\ & - \tfrac{4}{3}(p_1 - p_2)^2 F(h, q), \end{aligned} \tag{6}$$

where

$$F(h, q) = \sum_{k=1}^{h-3} k(k+1)(k+2)q^{h-3-k}.$$

The nonpolynomial function $F(h, q)$ monotonically increases when q belongs to the open interval (0, 1). Thus $F(h, 0) \leqslant F(h, q) \leqslant F(h, 1)$ with

$$F(h, 0) = (h-1)(h-2)(h-3)$$

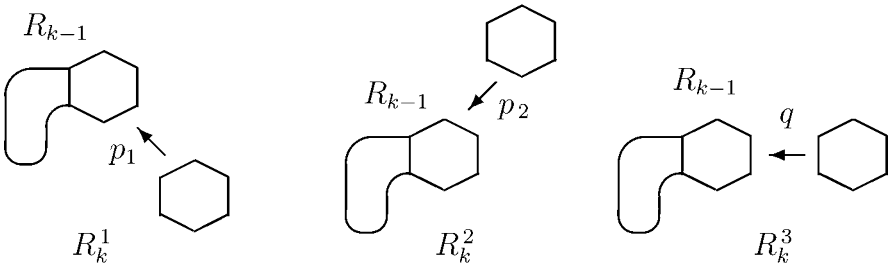

Figure 10. Growth of a random hexagonal chain R_h.

and

$$F(h, 1) = h(h-1)(h-2)(h-3)/4.$$

If $h \to \infty$ and $q \neq 1$, then

$$\lim_{h\to\infty} F(h, q)/h^3 = 1/(1-q)$$

and

$$W_h \sim [4 + 4q/3 - 4(p_1 - p_2)^2/3(1-q)]h^3,$$

i.e., W_h is asymptotically cubic in h.

5. Formulas for Classes of Hexagonal Systems

In this section we provide more expressions for the Wiener index of catacondensed systems and hexagonal chains. For these classes, formulas for calculating W reflect the pattern of branching. Some conditions for the coincidence of Wiener indices are also established.

5.1. HEXAGONAL CHAINS

A hexagonal chain G consists of an ordered sequence of segments $S_1, S_2, \ldots, S_n$, $n \geqslant 1$, of lengths $\ell(S_i) = \ell_i$, where $h_G = \ell_1 + \ell_2 + \cdots + \ell_n - n + 1$. Let the hexagonal systems G_1 and G_2 be obtained from a chain G by deleting a segment S, that is, G_1 and G_2 are the connected components of $G \setminus S$. The number of hexagons of G_1 and G_2 will be denoted by $h_1 = h_1(S)$ and $h_2 = h_2(S)$, respectively. For every segment S, $h_G = h_1 + h_2 + \ell(S)$.

A type of segment will be coded by a binary indicator that describes the mutual relation of the segments. An element $z_i = z(S_i)$, either 0 or 1, is assigned to every segment S_i. We first set $z_1 = z_n = 0$. If S_i, $2 \leqslant i \leqslant n-1$, is a zigzag segment, then $z_i = 1$, otherwise $z_i = 0$. The system G in Figure 11 has one nonterminal zigzag segment of length 4 and indicators 0, 0, 1, 0, 0. The set of all nonzigzag segments of a hexagonal chain G is denoted by $\Omega(G)$.

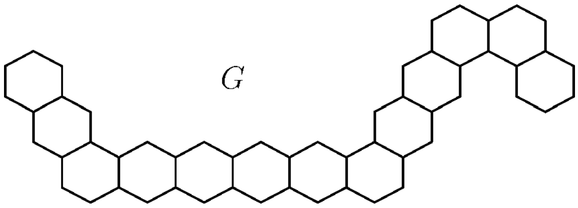

Figure 11. Hexagonal chain G with $W(G) = 13123$.

Let G be an arbitrary chain from HC_h described by parameters

$$L(G) = (\ell_1, \ell_2, \ldots, \ell_n) \quad \text{and} \quad Z(G) = (z_1, z_2, \ldots, z_n).$$

It is clear that these uniquely determine a system having n segments. Then the Wiener index of G may be calculated from these structural parameters [24].

THEOREM 5.1. *Let G be a hexagonal chain with segment lengths* $\ell_1, \ell_2, \ldots, \ell_n$ *and parameters* $z_1, z_2, \ldots, z_n$. *Then*

$$\begin{aligned} W(G) &= \sum_{i=1}^{n} W(L_{\ell_i}) - 27(n-1) + \\ &\quad + 16 \sum_{i=1}^{n} \left((\ell_i - 1) \sum_{k=i+1}^{n} \left[(\ell_i + \ell_k + 1)(\ell_k - 1) + \right.\right. \\ &\qquad \left.\left. + (2\ell_k - 3 + z_k) \sum_{j=k+1}^{n} (\ell_j - 1) \right] \right). \end{aligned} \tag{7}$$

Segments may be regarded as elementary bricks of a chain. Equation (7) summarizes the contribution of all these bricks to the Wiener index. If a chain has a large number of segments then the calculation of W by means of this formula becomes tedious. The above result was used for establishing a congruence relation between W-values of hexagonal chains ([23]).

The next formula shows that zigzag and nonzigzag segments make different contributions to the Wiener index.

THEOREM 5.2. *Let G be an arbitrary element of* HC_h *with segment lengths* $\ell_1, \ell_2, \ldots, \ell_n$. *Then*

$$W(G) = W(L_h) - 16 \sum_{S \in \Omega(G)} h_1 h_2 - 4 \left(h^2 + n - 1 - \sum_{i=1}^{n} \ell_i^2 \right), \tag{8}$$

where the first summation goes over all nonzigzag segments of G.

Consider, for instance, the hexagonal chain G depicted in Figure 11. This chain has $h = 13$ hexagons and $n = 5$ segments with lengths 3, 6, 4, 2, 2. Two nonzigzag segments have lengths 6 and 2. Since $W(L_{13}) = 13859$, we immediately arrive at

$$\begin{aligned} W(G) &= 13859 - 16(2 \cdot 5 + 10 \cdot 1) - 4[169 + 5 - 1 - \\ &\quad - (9 + 36 + 16 + 4 + 4)] = 13123. \end{aligned}$$

Equation (8) can be applied to completely describe the Wiener index of chains having n segments (say, $n = 4$) of equal length ℓ, $\ell \geqslant 2$. The class EHC_h consists of three systems with $h = 4\ell - 3$ hexagons (cf. Section 2). After elementary calculation, we obtain

$$\begin{aligned} W(G_1) &= (16h^3 + 27h^2 + 44h - 6)/3, \\ W(G_2) &= (16h^3 + 21h^2 + 56h - 12)/3, \\ W(G_3) &= (16h^3 + 15h^2 + 68h - 18)/3. \end{aligned}$$

Using formula (8), one can easily derive the extremal values of the Wiener index of fibonacenes, hexagonal chains with equal segments, and hexagonal systems with a given number of angularly connected hexagons given in Section 2. For example, $\Omega(G) = 0$ for a fibonacene G with maximum W; a zigzag chain with minimum W has segments of lengths $\ell_i = 2$ for all i.

Equation (8) also implies simple necessary and sufficient conditions for certain hexagonal chains to have the same Wiener index. Let $ZHC_{h,n}$ be the subset of ZHC_h in which every element (a zigzag chain) consists of n segments. Denote a sequence of segment lengths of hexagonal chains G and G' by $(\ell_1, \ell_2, \dots, \ell_n)$ and $(\ell'_1, \ell'_2, \dots, \ell'_{n'})$, respectively.

COROLLARY 5.2.1 *Let G and G' be arbitrary hexagonal chains with n segments. Then $W(G) = W(G')$ if and only if $\sum_{i=1}^{n} \ell_i^2 = \sum_{i=1}^{n} \ell_i'^2$.*

Consider two sequences of segment lengths $(k + 2, k + 5, k + 5)$ and $(k + 3, k + 3, k + 6)$, where $k \geqslant 0$. These sequences generate an infinite number of pairs of hexagonal chains satisfying the above condition. Indeed, the corresponding chains have $h = (3k + 12) - 3 + 1 = 3k + 10$ hexagons and the equalities $\sum_{i=1}^{3} \ell_i^2 = \sum_{i=1}^{3} \ell_i'^2 = 3k^2 + 24k + 54$ hold. It is easy to find chains having even number of segments and the same W, for instance, $(k - 5, k, k, k + 5)$ and $(k - 4, k - 3, k + 3, k + 4)$ for $k \geqslant 7$.

If chains contain different number of segments, then the coincidence of W depends on the relation between the number of segments and their lengths.

COROLLARY 5.2.2 *Let $G \in ZHC_{h,n}$ and $G' \in ZHC_{h,n'}$. Then $W(G) = W(G')$ if and only if $\sum_{i=1}^{n} \ell_i^2 - \sum_{i=1}^{n'} \ell_i'^2 = n - n'$.*

An example of elements of $ZHC_{7,2}$ and $ZHC_{7,3}$ can be obtained from the sequences of segment lengths (4, 4) and (2, 2, 5). The sequences $(3, k, k)$ and (2, 2,

$k-1, k+1)$ define an infinite family of hexagonal chains satisfying the last corollary. For these systems, $h = 2k+1$ and $\sum_{i=1}^{4} l_i^2 - \sum_{i=1}^{3} l_i'^2 = (2k^2+10) - (2k^2+9) = 1$.

The following method allows the construction of more systems having the same Wiener index.

COROLLARY 5.2.3 *Let $G, G' \in HC_h$ where G' is obtained from G by interchanging two neighboring zigzag segments. Then $W(G) = W(G')$.*

The smallest chains to which Corollary 5.2.3 is applicable have five hexagons and the sequences of segment lengths (2, 2, 3) and (2, 3, 2). Suppose that all segments of an element of $ZHC_{h,n}$ have mutually different lengths. Applying Corollary 5.2.3, one can obtain $n!/2$ nonisomorphic chains having equal W. It should be noted that it is also admissible to change the position of zigzag segments between any neighboring nonzigzag segments in a hexagonal chain.

5.2. CATACONDENSED HEXAGONAL SYSTEMS

In this section, we consider hexagonal systems from *CHS*. These, by definition, may possess branched hexagons, i.e., hexagons having three neighboring hexagons.

We distinguish between two types of branchings in a catacondensed hexagonal system. The first type of branching pertains to a single branched hexagon. The corresponding configuration may be described by three subgraphs G_1, G_2 and G_3 attached to the branching hexagon r, as shown in Figure 12. We associate with the hexagon r three quantities h_1, h_2 and h_3 that are the number of hexagons in the subgraphs G_1, G_2 and G_3, respectively.

The below considerations can be directly extended to the case when one of the subgraphs G_i, $i = 1, 2, 3$, is empty (when, of course, the hexagon r is not branched whereas the respective catacondensed system may, but need not, be branched). It just has to be assumed that $h_i = 0$ if the subgraph G_i is empty.

Denote by $B(G)$ the set of all hexagons of mode A and all branched hexagons in a catacondensed hexagonal system G.

The second type of branching is defined by two hexagons r and r' of $B(G)$, such that no hexagon of G being between r and r' belongs to $B(G)$. The corresponding configuration includes four subgraphs G_4, G_5 and G_4', G_5' as depicted in Figure 12; any of these subgraphs may also be empty. Let h_4, h_5, h_4' and h_5' be the number of hexagons of these subgraphs. Note that G_4 and G_5 are assumed to lie on the same side of the line crossing the centers of the hexagons between r and r'.

The following result shows that the Wiener index for every $G \in CHS_h$ can be calculated through $W(L_h)$ and configurations of branching in G [26].

THEOREM 5.3. *Let $G \in CHS_h$. Then*

$$W(G) = W(L_h) - 8\Bigg(5 \sum_{r\in B(G)} h_1h_2h_3 - \sum_{r\in B(G)} (h_1-1)(h_2-1)(h_3-1) +$$

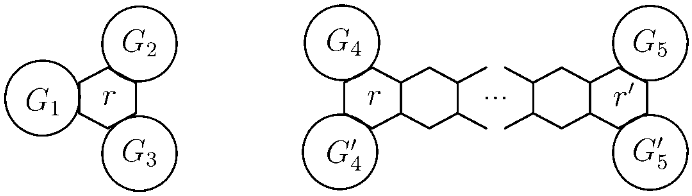

Figure 12. Types of branching in hexagonal systems of CB_h.

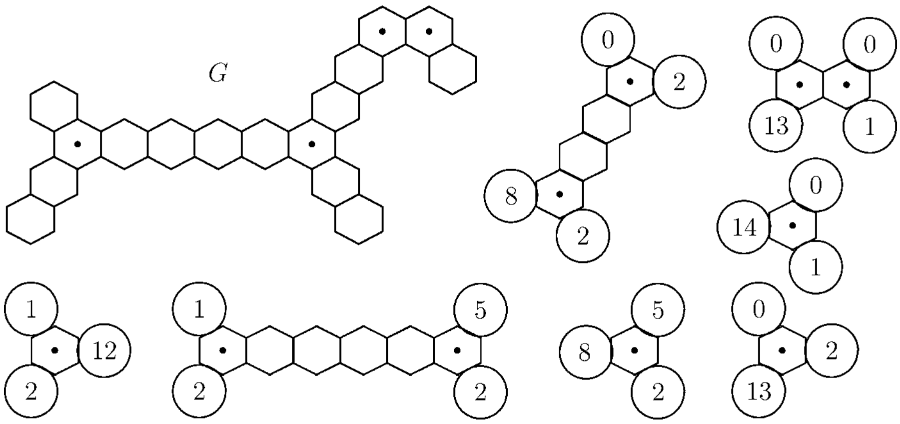

Figure 13. Hexagonal system G and its branchings.

$$+ \sum_{r,r' \in B(G)} (h_4 - h_4')(h_5 - h_5') + |B(G)|(h-2)\Bigg), \tag{9}$$

where the last summation goes over all neighboring hexagons of $B(G)$ in G.

Since branching hexagons can easily be recognized in a hexagonal system, formula (9) provides a convenient paper-and-pencil method for the calculation of the Wiener index.

As an illustration consider $G \in CHS_{16}$ depicted in Figure 13. This system has two branched hexagons and two hexagons of mode A marked by heavy dots, i.e. $|B(G)| = 4$. Configurations of all branchings are also given in Figure 13. Since $W(L_{16}) = 25057$, we immediately arrive at

$$\begin{aligned} W(H) &= W(L_{16}) - 8[5(1 \cdot 2 \cdot 12 + 2 \cdot 5 \cdot 8) - (1 \cdot 4 \cdot 7 + (-1) \cdot 1 \cdot 12) + \\ &\quad + (1-2)(5-2) + (0-2)(8-2) + (13-0)(1-0) + 4 \cdot 14] \\ &= 25057 - 8[520 - 16 - 3 - 12 + 13 + 56] = 20593. \end{aligned}$$

A *hexagonal star* is a branched catacondensed system having a single branched hexagon to which three (linear) segments are attached. Using Equation (9), the search for hexagonal stars with equal Wiener indices is reduced to numeric computation. If a hexagonal star S has segment lengths $\ell_i + 1$, $i = 1, 2, 3$, then

$$W(S) = W(L_h) - 8(4\ell_1\ell_2\ell_3 + \ell_1\ell_2 + \ell_1\ell_3 + \ell_2\ell_3).$$

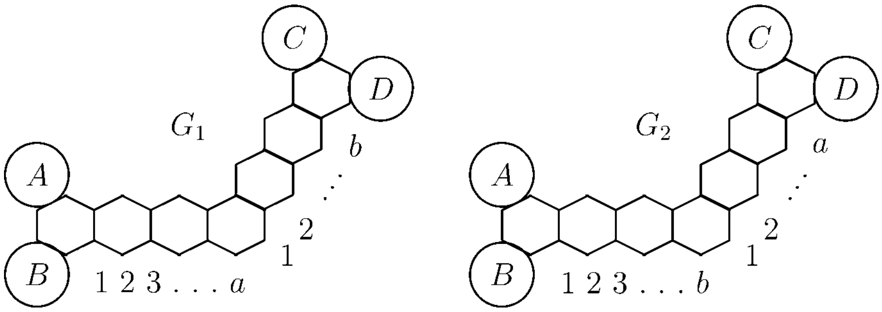

Figure 14. Hexagonal system with interchanged segments.

For $h \leqslant 40$, there are exactly 12 pairs of hexagonal stars with coinciding Wiener indices. The minimal systems have $h = 26$ and and have segment lengths 2, 5, 21 and 3, 3, 22.

For hexagonal chains, the above formula reduces to

COROLLARY 5.3.1 *Let $G \in HC_h$. Then*

$$W(G) = W(L_h) - 8\Bigg(\sum_{r\in B(G)} h_1h_2 + \sum_{r,r'\in B(G)} (h_4 - h_4')(h_5 - h_5')\Bigg).$$

We do not know simple conditions for the coincidence of Wiener indices for branched catacondensed systems. However, a coincidence can be deduced in some special cases. Consider, for instance, systems G_1 and G_2 with segments of length a and b, $a \neq b$, shown in Figure 14. These systems have the same structure except the position of two segments. Applying Equation (9), we have

$$W(G_1) - W(G_2) = 2(a - b)(h_A - h_C),$$

i.e., this difference does not depend on the subgraphs B and D. Therefore, $W(G_1) = W(G_2)$ if and only if $h_A = h_C$. If $h_A = h_C = 0$, then the segments are zigzag ones.

COROLLARY 5.3.2 *Let G_1, $G_2 \in CHS_h$ and G_2 be obtained from G_1 by interchanging two neighboring zigzag segments. Then $W(G_1) = W(G_2)$.*

Note that the Wiener index of the linear chain L_h with $p = 4h + 2$ vertices may be presented as follows

$$\begin{aligned} W(L_h) &= \frac{1}{2}\binom{4h+4}{3} - 1 = \frac{1}{2}\binom{p+2}{3} - 1 \\ &= \frac{1}{2}\left[\binom{p}{3} + 2\binom{p}{2} + \binom{p}{1}\right] - 1. \end{aligned}$$

This implies some analogy between Equation (9) of hexagonal systems and a combinatorial formula for calculating W of trees in [44].

5.3. PERICONDENSED HEXAGONAL SYSTEMS

It seems that the first explicit formulas for series of simple pericondensed systems were derived in [3]. On the other hand, Theorem 3.1 enables us to derive a general method by means of which many explicit formulas can be derived.

Let G be a hexagonal system. Recall (see the text after Theorem 3.1) that we can partition the edge set of G into edge-subsets $E_1, E_2, \ldots, E_k$ such that the graphs $G_i = G \setminus E_i$, $i = 1, 2, \ldots, k$, consist of two connected components G_i^0 and G_i^1. Let $p_i^0 = |G_i^0|$ and $p_i^1 = |G_i^1|$. Then, based on Theorem 3.1, we can derive [61]:

THEOREM 5.4. *Let G be a hexagonal system. Then $W(G) = \sum_{i=1}^{k} p_i^0 p_i^1$.*

This theorem was applied in [61] to the members C_k of the circumcoronene series, resulting in the earlier-mentioned formula (2). The same formula was independently, and by completely other means, obtained in [108]. Based on Theorem 5.4, formulas were derived for the Wiener index of a variety of families of symmetric pericondensed hexagonal systems: parallelograms, trapeziums, bitrapeziums, triangles, several parallelogram-like and hexagon-like hexagonal systems, ... [86]. For instance, if $T(n, k)$ denotes the trapezium hexagonal system with n columns and k rows of hexagons, then we have

$$\begin{aligned} W(T(n,k)) &\\ = \frac{4n^3(k^2+2k+1)}{3} &- \frac{2n^2(k+1)(2k^2-8k-3)}{3} + \\ &+ \frac{2n(k^4-4k^3+6k^2+9k+1)}{3} - \frac{k(8k^4+35k^2-45k-28)}{30}. \end{aligned}$$

After the publication of Theorem 5.4 (in [61]) Shiu and Lam arrived at an equivalent result [109] which they also used for obtaining formulas for W of various classes of pericondensed hexagonal systems. Some other aspects and applications of Theorem 5.4 are outlined in [52, 68, 82, 88, 121].

6. Properties of Values of the Wiener Index

Searching for nonisomorphic graphs with the same values of a graph invariant is a traditional direction of research in graph theory. In chemical graph theory the set of W-values of hexagonal systems have been subject to detailed investigation of this kind since a good ability of an invariant to distinguish between nonisomorphic graphs is important for applications.

6.1. CONGRUENCE RELATIONS FOR THE WIENER INDEX

In this section we consider catacondensed systems. Let G be a connected bipartite graph with parts A and B. Clearly, $d(u, v)$ is even if both vertices u and v belong to the same part; otherwise $d(u, v)$ is odd. This immediately implies that $d_G(v) \equiv 1 \pmod 2$ if and only if either $v \in B$ and $|A|$ is odd or $v \in A$ and $|B|$ is odd. Further, $W(G) \equiv 1 \pmod 2$ if and only if both $|A|$ and $|B|$ are odd. For any catacondensed hexagonal system, both $|A|$ and $|B|$ are odd ([2]). By this, we have the first result restricting the possible values of the Wiener index ([41, 42]).

THEOREM 6.1. *If v is a vertex of a catacondensed system G, then $d_G(v) \equiv 1 \pmod 2$. For any catacondensed system G, $W(G) \equiv 1 \pmod 2$, i.e., $W(G)$ is an odd number.*

This result eliminates half of possible values of the Wiener index. However, a much stronger result applies ([41, 42]):

THEOREM 6.2. *Let $G_1, G_2 \in CHS_h$. Then $W(G_1) \equiv W(G_2) \pmod 8$, i.e., the difference $W(G_1) - W(G_2)$ is divisible by 8.*

Examples show that the above result is the best possible unconditional congruence relation for systems of this class. Some relations with stronger conditions have been derived from Equation (7) of Theorem 5.1 for some subclasses of hexagonal chains ([24]). A typical such statement is

THEOREM 6.3. *If hexagonal chains G_1 and G_2 have coinciding sets of segment lengths $\{\ell_1, \ell_2, \ldots, \ell_n\}$ and $\ell_i = kc_i + 1$ for all $i = 1, 2, \ldots, n$ ($k \geqslant 1$, $c_i \geqslant 1$), then $W(G_1) \equiv W(G_2) \pmod{16k^2}$.*

COROLLARY 6.3.1 *Let $G_1, G_2 \in EHC_h$ with segments of length ℓ. Then $W(G_1) \equiv W(G_2) \pmod{16(\ell - 1)^2}$.*

Since $FHC_h \subset EHC_h$, the relation $W(G_1) \equiv W(G_2) \pmod{16}$ in particular holds for arbitrary fibonacenes G_1 and G_2 with equal number of hexagons.

Let $n(G)$ be the number of all segments in $G \in CHS_h$. Then $n(G) = n_o(G) + n_e(G)$, where $n_o(G)$ and $n_e(G)$ denote the number of segments of odd and even length, respectively. If a segment has odd or even length, then it is said to be *even* or *odd*, respectively. The following congruence relation was obtained from Equation (7) for hexagonal chains having equal number of segments ([23]).

THEOREM 6.4. *Let G_1 and G_2 be hexagonal chains with the same number of segments. Then $W(G_1) \equiv W(G_2) \pmod{16}$ if and only if $n_o(G_1) \equiv n_o(G_2) \pmod 4$.*

The next result shows the main role of even segments in the case of general catacondensed systems. Namely, new necessary and sufficient conditions for modulo 16 rule have been formulated in terms of even segments ([25]). The number of odd segments does not influence this property of W (the previous theorem can be equivalently reformulated in terms of even segments).

THEOREM 6.5. *Let* $G_1, G_2 \in CHS_h$. *Then* $W(G_1) \equiv W(G_2) \pmod{16}$ *if and only if* $n_e(G_1) \equiv n_e(G_2) \pmod 4$.

The number of hexagons h and the number of even segments $n_e(G)$ always have different parity. Indeed, suppose that segments S_1 and S_2 are obtained from a segment S by a kink transformation, $S \to S_1S_2$. Then the change of segments' parity is described by one of the cases $E \to EO$, $E \to OE$, $O \to OO$ or $O \to EE$, where E and O indicate the parity of the segments. A hexagonal system with an even number of hexagons has at least one even segment.

The above congruence relation immediately leads to a necessary condition for the coincidence of W-values of catacondensed hexagonal systems.

COROLLARY 6.5.1. *Let* $G_1, G_2 \in CHS_h$. *If* $W(G_1) = W(G_2)$, *then* $n_e(G_1) - n_e(G_2)$ *is divisible by* 4.

The obtained congruence relation induces decomposition of the set CHS_h into four disjoint subsets C_0, C_1, C_2, and C_3, such that an element of C_i contains $4k+i$, $k \geqslant 0$, even segments. Then $W(G_1) \neq W(G_2)$ if $G_1 \in C_i$ and $G_2 \in C_j$ with $i \neq j$.

If the systems considered have segments with prescribed lengths, then the congruence relation may be strengthened.

THEOREM 6.6. *Let the systems* $G_1, G_2 \in CHS_h$ *have segment length* $\{\ell_1, \ell_2, \dots, \ell_n\}$ *and* $\{\ell'_1, \ell'_2, \dots, \ell'_n\}$, *where* $\ell_i = ka_i + 1$ *and* $\ell'_i = kb_i + 1$, $i \geqslant 1$, $k \geqslant 2$. *Then* $W(G_1) \equiv W(G_2) \pmod{8k^2}$.

Note that this result does not contain conditions on the number of even segments (but it also does not provide congruence modulo 16). The congruence modulo 32 is valid for subclasses of hexagonal systems corresponding to even values of k [25].

COROLLARY 6.6.1. *Let* $G_1, G_2 \in CHS_h$ *and let all their segments be odd* (*when also h must be odd*). *Then* $W(G_1) \equiv W(G_2) \pmod{32}$.

There are no known congruence relations for pericondensed hexagonal systems.

6.2. NONREALIZABLE VALUES OF THE WIENER INDEX

The determination of the ranges of nonrealizable values of a graph invariant may prove useful in applications, namely, for solving the inverse problem in prediction of properties of chemical compounds and design of compounds with desired properties; for details, see [115].

In this section we restrict our considerations to hexagonal chains and simple hexagonal chains. First consider graphs from HC_h (for graphs of sHC_h, we must take the snake instead of the helix).

In view of Theorem 6.2 and the fact that linear chains and helixes are extremal for hexagonal chains, define a set of possible values of the Wiener index of hexagonal chains with h hexagons as

$$P_h = P(HC_h) = \{W(H_h) + 8n \mid n = 0, 1, \ldots, \tfrac{1}{8}[W(L_h) - W(H_h)]\}.$$

The set P_h is a discrete interval of odd numbers of cardinality $|P_h| = h(2h^2 - 9h + 13)$. Denote by

$$W_h = W(HC_h) = \{W(G) \mid G \in HC_h\}$$

the set of W-values for all elements of HC_h. Then the set of nonrealizable values of W is defined as

$$E_h = E(HC_h) = P_h \setminus W_h.$$

It is known that {2, 3, 5, 6, 7, 11, 12, 13, 15, 17, 19, 33, 37, 39} is the set of non-realizable values of bipartite graphs ([71]). The following result shows that (except in the trivial cases of $h = 1$ and $h = 2$) there are nonrealizable values in the case of the Wiener index of hexagonal systems ([17, 19]).

THEOREM 6.7. *For every $h \geqslant 4$, $E_h \neq \emptyset$. The set of nonrealizable values from P_h may be represented as $E_h = \bigcup_i [a_i, b_i]$, where some of these discrete subintervals have cardinalities linear in h.*

The longest intervals of nonrealizable values are placed at the ends of P_h. Their lengths are equal to $h - 3$ and $h - 5$ (at the left end of P_h) and $2h - 12$ and $2h - 7$ (at the right end of P_h).

Tables I and II contain data on intervals of possible and nonrealizable values of the Wiener index for elements of HC_h and sHC_h, respectively (S_h denotes the serpent with h hexagons). The first number in the sixth column is equal to $|E_h|$ and the second number $\#I_h$ counts the number of intervals of nonrealizable values, i.e., this ratio is equal to the average cardinality of such intervals. By definition, $|W_h| = |P_h| - |E_h|$. Detailed numeric information for all nonrealizable intervals of P_h for $h \leqslant 16$ can be found in [17].

Because of the existence of nonrealizable values, the following question arises: can a value of P_h be realized by a hexagonal system with different number of hexagons? It was shown that the numbers of hexagons must satisfy the following relation ([18]).

THEOREM 6.8. *Let $G_1 \in HC_{h_1}$, $G_2 \in HC_{h_2}$ and $h_1 \neq h_2$. If $W(G_1) = W(G_2)$, then $h_{G_1} \equiv h_{G_2} \pmod 4$.*

Combining the above result with the expressions for the extremal values of the Wiener index, one obtains an additional restriction on h.

Table I. Structure of W-values for hexagonal chains

h	$\|HC_h\|$	$W(H_h)$	$W(L_h)$	$\|P_h\|$	$\|E_h\|/\#I_h$	$\|W_h\|$
1	1	27	27	1	0	1
2	1	109	109	1	0	1
3	2	271	279	2	0	2
4	4	529	569	6	2/2	4
5	10	899	1011	15	6/3	9
6	25	1397	1637	31	13/6	18
7	70	2039	2479	56	21/9	35
8	196	2841	3569	92	25/7	67
9	574	3819	4939	141	36/10	105
10	1681	4989	6621	205	45/13	160
11	5002	6367	8647	286	56/15	230
12	14884	7969	11049	386	67/16	319
13	44530	9811	13859	507	80/19	427
14	133255	11909	17109	651	93/19	558
15	399310	14279	20831	820	113/23	707
16	1196836	16937	25057	1016	128/28	888

Table II. Structure of W-values for simple hexagonal chains

h	$\|sHC_h\|$	$W(S_h)$	$W(L_h)$	$\|P_h\|$	$\|E_h\|/\#I_h$	$\|W_h\|$
1	1	27	27	1	0	1
2	1	109	109	1	0	1
3	2	271	279	2	0	2
4	4	529	569	6	2/2	4
5	10	899	1011	15	6/3	9
6	24	1445	1637	25	8/5	17
7	67	2135	2479	44	12/7	32
8	182	2985	3569	74	17/4	57
9	520	4107	4939	105	17/6	88
10	1474	5241	6621	151	23/9	128
11	4248	6943	8647	214	33/10	181
12	12196	8833	11049	278	32/12	246
13	35168	10963	13859	363	41/15	322
14	101226	13349	17109	471	51/13	420
15	291565	16199	20831	580	54/16	526
16	838764	19337	25057	716	61/17	655

Table III. Nonempty common intervals of the Wiener index

$h-4$	h	$\lvert HC_{h-4}\rvert$	$\lvert HC_h\rvert$	$\lvert P_{h-4}\rvert$	$\lvert P_h\rvert$	$\lvert P_{h-4} \cap P_h\rvert$
23	27	2615147350	212822683802	3312	5526	211
24	28	7845353476	635467254244	3796	6202	467
25	29	23535971854	1906400965570	4325	6931	760
26	30	70607649841	5719200505225	4901	7715	1092
27	31	211822683802	17157599124190	5526	8556	1465
28	32	635467254244	51472790198116	6202	9456	1881
29	33	1906400965570	154418363419894	6931	10417	2342
30	34	5719200505225	463255068736321	7715	11441	2859

COROLLARY 6.8.1 *Let two arbitrary hexagonal chains belong to the classes HC_h and HC_{h+4}. If $h \leqslant 22$ then $P_h \cap W_{h+4} = \emptyset$ and, therefore, these systems have distinct Wiener indices.*

This result demonstrates that in order to obtain intervals of nonrealizable values for hexagonal chains up to 22 hexagons, we need simply to join all such intervals for each $h \leqslant 22$.

COROLLARY 6.8.2 *Let two arbitrary hexagonal chains belong to the classes sHC_h and sHC_{h+4}. If $h \leqslant 23$ then $P_h \cap W_{h+4} = \emptyset$ and these chains have distinct Wiener indices. For elements of jHC_h and jHC_{h+4}, the corresponding bound is $h \leqslant 33$.*

Since the Wiener index of a graph considerably depends on the number of vertices, a greater number of hexagons of an element of HC_{h+4} should be compensated by smaller distances between its vertices than those in a system from the class HC_h. So we can expect a system from HC_{h+4} to be similar to the helix H_{h+4} and a system from HC_h to be similar to the linear chain L_h.

If the cardinality of the set $P_h \cap P_{h+4}$ is small, then systems whose Wiener index belongs to this set may not exist at all, since the set may be contained in the set of nonrealizable elements. Table III contains information about smallest nonempty intervals $P_{h-4} \cap P_h$. By means of computer calculation, several pairs of hexagonal chains of different size having the same W were found. Minimal known hexagonal systems with the same Wiener indices belong to sHC_{25} and jHC_{29} (see systems G_1 and G_2 in Figure 15) and $W(G_1) = W(G_2) = 89059$. The simple systems G_3 and G_4 from sHC_{40} and sHC_{36} with $W(G_3) = W(G_4) = 262057$ are also depicted in Figure 15. Other examples can be found in [17–19].

Graph invariants encountered in chemical studies generally reflect the structure of molecules and are regarded as structure-descriptors. Therefore it is desirable to

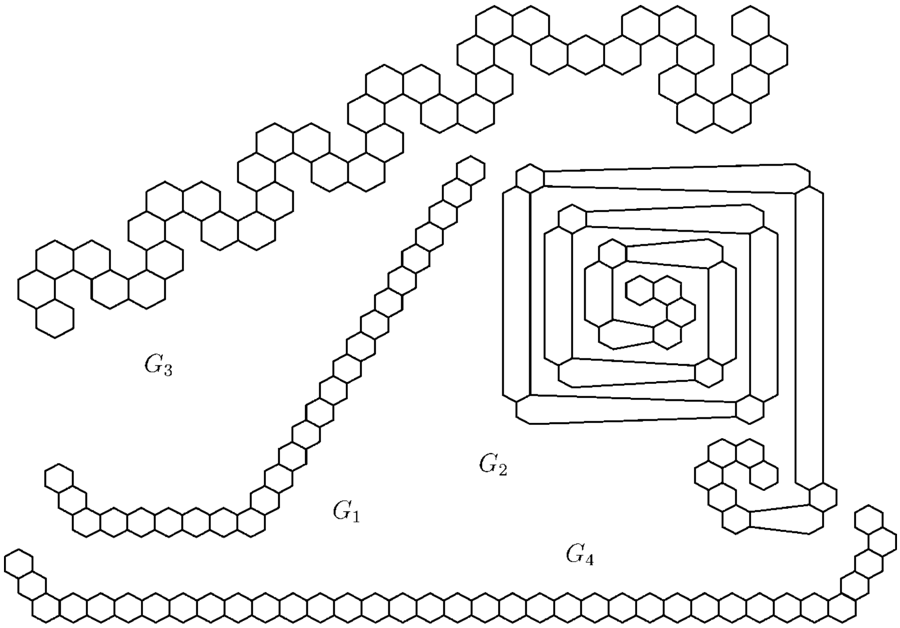

Figure 15. Hexagonal chains with equal W and different number of hexagons.

have a high isomer-discriminating power, namely that for nonisomorphic molecular graphs with a constant number of vertices and edges, the invariant in question assumes different numerical values ([91, 104, 105]). The ability of a graph invariant to discriminate between isomers is called its *discriminating ability*. One can always find families of graphs with fixed numbers of vertices and edges such that their Wiener index has the same value for all members of the family [70].

The discriminating ability of a graph invariant GI on a set of graphs U is usually expressed in terms of its *mean isomer degeneracy*,

$$I = \frac{|U|}{|\{GI(G) \mid G \in U\}|}.$$

Another, equivalent, way of expressing the same property is by means of the *isomer-discriminating power* which is equal to $1/I$.

By a *degeneracy class* of a number from P_h we will mean the subset of HC_h consisting of all graphs with this number. The quantity I may be regarded as the average size of the degeneracy classes. The cardinality of the set HC_h grows as 3^h, while the number of possible elements of P_h grows only as h^3. Therefore, for each possible value of P_h, the average cardinality of the corresponding degeneracy class has exponential growth. Since the set P_h contains nonrealizable values, the ratio $|HC_h|/|P_h|$ is the lower bound for the size of real average class $I = |HC_h|/|W_h|$. The discriminating ability of the Wiener index for hexagonal systems was studied in [17, 65, 91, 92, 114]. Diagrams of hexagonal chains up to $h = 12$ hexagons from the maximal degeneracy classes can be found in [17].

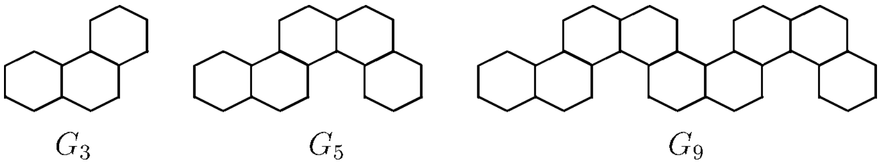

Figure 16. Hexagonal systems G for which $W(G) = W_h = W_{\text{avr}}$.

6.3. PROPERTIES OF THE WIENER INDEX OF FIBONACENES

In this section two unexpected properties of fibonacenes will be explained [35]. Define the average value of the Wiener index with respect to FHC_h as

$$W_{\text{avr}}(FHC_h) = \frac{1}{|FHC_h|} \sum_{G \in FHC_h} W(G).$$

The number of fibonacenes $|FHC_h|$ is equal to $2^{h-4} + 2^{\lfloor (h-4)/2 \rfloor}$.

THEOREM 6.9. $\sum_{G \in FHC_h} W(G) \equiv 0 \pmod{|FHC_h|}$, *i.e., the sum of all the Wiener indices of all h-hexagon fibonacenes is divisible by the number of these systems.*

The above result does not reflect the property of Wiener index of any particular fibonacene, but a collective property of all such chains.

This also implies that $W_{\text{avr}}(FHC_h)$ is an integer. Recall that fibonacenes are generated by means of the GKQ-algorithm for the case $q = 0$ (see Section 2). Denote by W_h the expected value of the Wiener index of the random hexagonal chain under such generation. Then we have another unexpected result:

COROLLARY 6.9.1 *For the class of fibonacenes, the two averages W_{avr} and W_h coincide*

$$W_{\text{avr}}(FHC_h) = W_h = 4h^3 + 16h^2 + 6h + 1.$$

Examples of the corresponding systems for odd h are shown in Figure 16. The Wiener index of these systems was found a long time ago ([67]). For some even h, $W_{\text{avr}}(FHC_h)$ is a nonrealizable value (at least for $h = 4, 6, 8, 12, 16$ ([35])).

7. Decomposition of the Wiener Index

A number of decompositions of the Wiener index were used to establish correlations between properties of chemical compounds and the parts of this index [40, 93–95].

7.1. DECOMPOSITION WITH RESPECT TO VERTEX DEGREE

We consider decomposition of W into sums of vertex distances defined by vertices' degree for catacondensed systems. The set of vertices of such a system can be divided into two disjoint subsets $V_2 = \{v \in V(G) | \deg(v) = 2\}$ and $V_3 = \{v \in V(G) | \deg(v) = 3\}$, where $|V_2| = 2(h+2)$ and $|V_3| = 2(h-1)$. Then the Wiener index of a hexagonal system G can be decomposed into two parts:

$$W(G) = \tfrac{1}{2}\left(\sum_{v \in V_2} d_G(v) + \sum_{v \in V_3} d_G(v)\right) = \tfrac{1}{2}(D_2(G) + D_3(G)). \qquad (10)$$

For the linear chain L_h, this decomposition yields

$$D_2(L_h) = \tfrac{2}{3}(8h^3 + 36h^2 + 31h + 6) \quad \text{and} \quad D_3(L_h) = \tfrac{2}{3}(8h^3 - 5h - 3).$$

The following far-reaching result has been established in [27]:

THEOREM 7.1. *Let G be an arbitrary catacondensed hexagonal system with h hexagons. Then $D_2(G) = D_2(L_h) - \Delta(G)$ and $D_3(G) = D_3(L_h) - \Delta(G)$, where $\Delta(G) > 0$ depends only on G.*

The quantity $\Delta(G)$ is determined by the changes of vertex distances under kink transformations transferring the linear chain to the graph G. If $W(G_1) = W(G_2)$, then $W(G_1) - W(G_2) = \Delta(G_2) - \Delta(G_1) = 0$, implying $\Delta(G_2) = \Delta(G_1)$. We thus arrive at a Corollary 7.1.1 which, earlier, was put forward as a conjecture ([20, 37]).

COROLLARY 7.1.1 *If $W(G_1) = W(G_2)$ for catacondensed systems G_1 and G_2, then $D_2(G_1) = D_2(G_2)$ and $D_3(G_1) = D_3(G_2)$.*

COROLLARY 7.1.2 *In order to check the coincidence of the Wiener index of catacondensed systems, it is sufficient to compare distance sums for vertices of degree 2 or of degree 3.*

Theorem 7.1 was used for establishing the relationship between the Wiener index and molecular topological index (see Section 8). It should be noted that Corollary 7.1.1 cannot be extended to pericondensed systems.

Consider another decomposition of the Wiener index into three parts for $G \in CHS$:

$$\begin{aligned} W(G) &= \tfrac{1}{2}\Bigg(\sum_{v,u \in V_2} d(v,u) + \sum_{v,u \in V_3} d(v,u) + \sum_{v \in V_2, u \in V_3} d(v,u) + \\ &\qquad + \sum_{v \in V_3, u \in V_2} d(v,u)\Bigg) \\ &= \tfrac{1}{2}(D_{22}(G) + 2D_{23}(G) + D_{33}(G)). \end{aligned}$$

Computer calculations support the following conjecture [20, 37].

CONJECTURE 7.2. *If* $W(G_1) = W(G_2)$ *for* $G_1, G_2 \in CHS_h$*, then* $D_{22}(G_1) = D_{22}(G_2)$*,* $D_{23}(G_1) = D_{23}(G_2)$*, and* $D_{33}(G_1) = D_{33}(G_2)$*.*

7.2. HOSOYA POLYNOMIAL

There is a natural decomposition of the Wiener index into groups of equidistant vertices. Denote by $d(G, k)$ the number of pairs of vertices of a graph G that are at distance k apart. Let $D(G)$ be the diameter of a graph G. Then the Wiener index of a (connected) graph G can be written in the form

$$W(G) = \sum_{k=1}^{D(G)} kd(G, k).$$

The sequence $(d(G, 0), d(G, 1), \ldots, d(G, D))$ is a well-known invariant in graph theory ([4]). Hosoya [76] proposed to consider this sequence in a polynomial form, that is now called the *Hosoya polynomial of* G:

$$H(G, x) = \sum_{k=1}^{D(G)} d(G, k)x^k.$$

Note that by the definition $d(G, 0) = p$ and $d(G, 1) = q$. The above two relations also immediately imply the main property (for our purposes) of the Hosoya polynomial: $H'(G, 1) = W(G)$, where H' denotes the first derivative of H.

In [64] expressions for the Hosoya polynomial for a number of periodic hexagonal chains are obtained and consequently also for their Wiener indices. In the sequel we describe the corresponding approach.

For a graph G, $k \geqslant 0$, and a vertex $v \in V(G)$, let $d(G, v, k)$ be the number of vertices of G at distance k from v. We set $d(G, v, 0) = 1$, and for $k < 0$, $d(G, v, k) = 0$. Define $H(G, v, x)$ as

$$H(G, v) \equiv H(G, v, x) = \sum_{k \geqslant 0} d(G, v, k)x^k.$$

Now we can state:

THEOREM 7.3. *Let the graph* G *be obtained by annelating a* 6*-cycle to the graph* G_0 *over an edge* (u, v)*. Then*

$$\begin{aligned} H(G, x) &= H(G_0, x) + (x + x^2)H(G_0, u, x) + (x + x^2)H(G_0, v, x) + \\ &\quad + 4 + 3x + 2x^2 + x^3. \end{aligned}$$

Theorem 7.3 provides a recursion that can be used for computing the Hosoya polynomial of catacondensed hexagonal systems. In order to do it, one also needs to recursively express the terms $H(G_0, u, x)$ and $H(G_0, v, x)$.

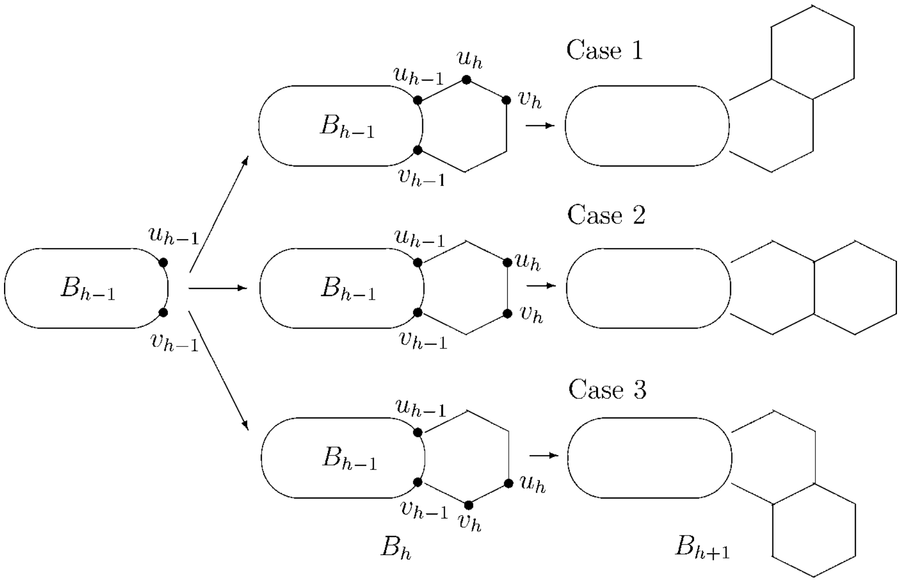

Figure 17. Three possible ways of attaching a hexagon to a hexagonal chain.

In the particular case of hexagonal chains Theorem 7.3 reduces to the following. Let G_h be a hexagonal chain with h hexagons obtained by adding a hexagon to G_{h-1} over an edge (u_{h-1}, v_{h-1}). Furthermore, let (u_h, v_h) be the edge that will be used in the subsequent annelation, that is, in the process $G_h \to G_{h+1}$. There are three possibilities for the edge (u_h, v_h) and these are shown in Figure 17.

Setting $\alpha_h \equiv H(G_h, x)$, $\beta_h \equiv H(G_h, u_h, x)$, and $\gamma_h \equiv H(G_h, v_h, x)$ we have

COROLLARY 7.2.1 *Let G_h be a hexagonal chain with h hexagons. Then the Hosoya polynomial α_h of G_h satisfies the following recurrence*

$$\alpha_h = \alpha_{h-1} + (x + x^2)(\beta_{h-1} + \gamma_{h-1}) + 4 + 3x + 2x^2 + x^3,$$

where $\alpha_0 = 2 + x$, $\beta_0 = \gamma_0 = 1 + x$. Moreover, β_h and γ_h obey the following recurrences, depending on the cases shown in Figure 17*:*

Case 1: $\beta_h = x\beta_{h-1} + 1 + x + x^2 + x^3$; $\gamma_h = x^2\beta_{h-1} + 1 + 2x + x^2$.
Case 2: $\beta_h = x^2\beta_{h-1} + 1 + 2x + x^2$; $\gamma_h = x^2\gamma_{h-1} + 1 + 2x + x^2$.
Case 3: $\beta_h = x^2\gamma_{h-1} + 1 + 2x + x^2$; $\gamma_h = x\gamma_{h-1} + 1 + x + x^2 + x^3$.

A hexagonal chain consisting of $n \geqslant 1$ hexagons can be constructed by a sequence of n annelations that can be straight, a 60-degree turn to the left, or a 60-degree turn to the right (relatively to the previous step); cf. Section 4.3 and Figure 10. This can be encoded by a string of length n over the alphabet $\{1, 2, 3\}$ where 1, 2, and 3 mean 'turn left', 'go straight', and 'turn right', respectively. Take any nonempty finite string s over $\{1, 2, 3\}$, and repeat it infinitely often to obtain the infinite string $S = sss\ldots$. Then S represents an infinite *periodic hexagonal chain* and the finite initial substrings of S represent an infinite family of finite periodic hexagonal chains. In [64], the Hosoya polynomial (and consequently the Wiener index) was explicitly computed for the following families of periodic hexagonal chains:

the linear chain: $s = 2$;
the helicene chain: $s = 1$;
the zigzag chain: $s = 13$;
the double-step zigzag chain: $s = 2123$;
the triple-step zigzag chain: $s = 221223$;
the double-step helicene: $s = 21$;
the triple-step helicene: $s = 221$; and
the no-name chains $s = 1133$, $s = 111333$, $s = 1122$, and $s = 111222$.

We list two examples. In the case of the helicene chain ($s = 1$), let G_n be the hexagonal chain represented by a string of n ones. Then $G_n = H_n$ and we have

$$\begin{aligned} H(H_n, x) \;=\; & \frac{1}{(x-1)^2}((x+1)^4 x^{n+2} + x^8 - 4x^6 - 4x^5 - \\ & - 3x^4 - 3x^3 - 2x^2 - 3x - \\ & - n(x-1)(x^2+1)(x^5 + 2x^4 + x^3 - x^2 + x + 4) + 2). \end{aligned}$$

From here we deduce

$$W(H_n) = H'(H_n, 1) = \tfrac{1}{3}(8n^3 + 72n^2 - 26n + 27)$$

a result already listed before. For the double-step zigzag chain ($s = 2123$), let G_n be the hexagonal chain represented by a string of n copies of 2123, so that G_n has $4n$ hexagons. For $n \geqslant 2$ we have:

$$\begin{aligned} H(G_n, x) \;=\; & \frac{1}{4(x-1)^2}(4(x+1)^2 x^{2n+1} - 5x^9 + 11x^7 - 3x^5 + \\ & + (-1)^n (x-1)^3 (x+1)^3 x^3 - 7x^3 - 8x^2 - 12x + \\ & + 2n(x-1)(x^2-2)(x^2+1)(x^4 + x^3 + x^2 + x + 4) + 8), \end{aligned}$$

and therefore

$$W(G_n) = H'(G_n, 1) = \tfrac{1}{3}(16n^3 + 24n^2 + 74n + 6(-1)^n - 51).$$

8. Relations Between Wiener Index and Other Invariants

8.1. MOLECULAR TOPOLOGICAL INDEX

The molecular topological index of a chemical graph G was put forward by Schultz [107]. It is defined as

$$MTI(G) = \sum_{i=1}^{p} \sum_{j=1}^{p} \deg(v_i)(A_{ij} + d_G(v_i, v_j)),$$

where A_{ij} is the element of the adjacency matrix of G. An entry A_{ij} is 1 if vertices i and j are adjacent and zero otherwise. The molecular topological index has found interesting chemical applications (for details, see [117]).

It has been demonstrated that *MTI* and W are closely mutually related for certain classes of molecular graphs, in particular, for trees ([47, 89]). Namely, if G is a tree on p vertices, then

$$MTI(G) = 4W(G) + \sum_{v \in V(G)} (\deg(v))^2 - p(p-1).$$

For hexagonal systems, the molecular topological index may be presented as follows [62]:

THEOREM 8.1. *Let $G \in HS_h$, possessing n_i internal vertices. Then*

$$MTI(G) = 4W(G) + \tfrac{1}{2}[4(13h-1) + 5n_i] + \sum_{\deg(v)=3} d(v).$$

For catacondensed systems, there is a simpler relation between *MTI* and W [29]:

THEOREM 8.2. *Let $G \in CHS_h$. Then*

$$MTI(G) = 5W(G) - (12h^2 - 14h + 5).$$

The proof of Theorem 8.2 is significantly based on the decomposition of the Wiener index into two parts as in Equation (10). The obtained formula immediately shows that W and *MTI* have the same discriminating ability.

COROLLARY 8.2.1 *Let $G_1, G_2 \in CHS_h$. Then $MTI(G_1) = MTI(G_2)$ if and only if $W(G_1) = W(G_2)$.*

Properties of the Wiener index imply also similar properties of the molecular topological index. For example, there is an unconditional regularity among *MTI*-values (for other relations see Section 6).

COROLLARY 8.2.2 *Let $G_1, G_2 \in CHS_h$. Then $MTI(G_1) \equiv MTI(G_2)$* (mod 40).

There are several estimates of *MTI* in terms of the Wiener index of simple hexagonal systems ([62, 83]). The sharpest bounds are given in the following result.

THEOREM 8.3. *Let G be a simple hexagonal system. Then*

$$\begin{aligned} &4W(G) + \lambda_1 W(G)^{2/3} + \lambda_2 W(G)^{1/3} - 15 \\ &\quad < MTI(G) < 6W(G) + \lambda_3 W(G)^{2/5} - \lambda_4 W(G)^{1/6}, \end{aligned}$$

where

$$\lambda_1 = (120/13)^{2/3} = 4.400\ldots, \qquad \lambda_2 = (120/104)^{1/3} = 1.048\ldots,$$

$$\lambda_3 = 9(45\sqrt{6}/32)^{2/5} = 14.760\ldots,$$

and

$$\lambda_4 = \sqrt{150}(120/13)^{1/6} = 17.738\ldots.$$

8.2. SZEGED INDEX

Let $e = (x, y)$ be an edge of a graph G. Let $n_1(e)$ be the number of vertices of G lying closer to x than to y and let $n_2(e)$ be the number of vertices of G lying closer to y than to x. A classical result in the theory of Wiener indices is the following. Let G be a tree. Then,

$$W(G) = \sum_{e \in E(G)} n_1(e) n_2(e). \tag{11}$$

For details see Theorem 8 in [30].

If G is not a tree then the right-hand side of Equation (11) needs not be equal to $W(G)$. Yet, the right-hand side of (11), namely

$$Sz(G) = \sum_{e \in E(G)} n_1(e) n_2(e)$$

is a well-defined quantity for all graphs and has been examined under the name *Szeged index*. The main properties of the Szeged index as well as an exhaustive list of references can be found in the review [54].

The Szeged index $Sz(G)$ of a hexagonal system G can be calculated by means of a formula analogous to the expression for $W(G)$ stated above as Theorem 5.4. Using the same notation as in Theorem 5.4 and denoting the number of edges in E_i by $|E_i|$, one has [60]

$$Sz(G) = \sum_{i=1}^{k} |E_i| p_i^0 p_i^1.$$

By means of this formula combinatorial expressions for the Sz-values of several classes of hexagonal systems were obtained ([48, 56]). A number of congruence relations for the Szeged indices of catacondensed hexagonal systems have been deduced that are fully analogous to what was described in Subsection 6.1 for the Wiener index ([31–33, 36, 81]).

9. Phenylenes and Hexagonal Squeezes

Phenylenes are a class of chemical compounds in which the carbon atoms form 6- and 4-membered cycles. Each 4-membered cycle (= square) is adjacent to two

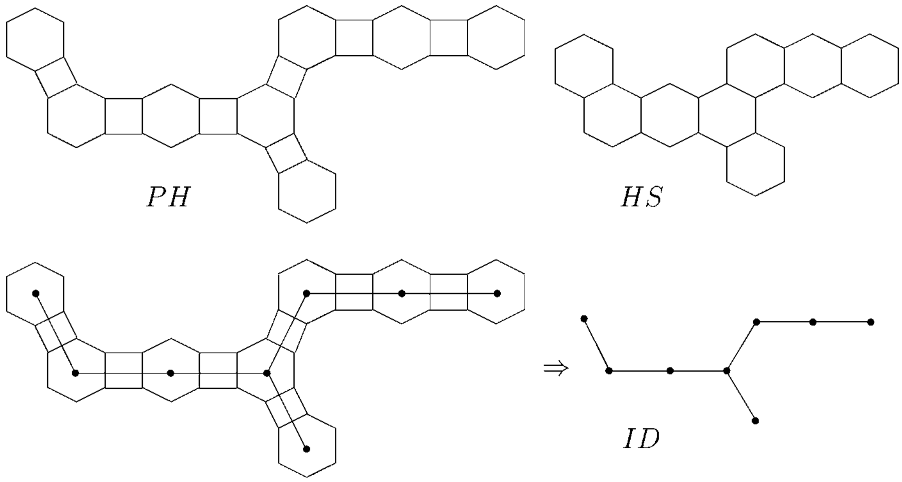

Figure 18. A phenylene (*PH*), its hexagonal squeeze (*HS*) and its inner dual (*ID*).

disjoint 6-membered cycles (= hexagons), and no two hexagons are adjacent. The respective molecular graphs are also referred to as *phenylenes*. Their structure (which we are not going to define in a rigorous manner) should be evident from the example depicted in Figure 18.

By eliminating,‘*squeezing out*’, the squares from a phenylene, a catacondensed hexagonal system (which may be jammed) is obtained, called the *hexagonal squeeze* of the respective phenylene ([45]). Clearly, there is a one-to-one correspondence between a phenylene (*PH*) and its hexagonal squeeze (*HS*). Both possess the same number (h) of hexagons. In addition, a phenylene with h hexagons possesses $h-1$ squares. The number of vertices of *PH* and *HS* is $6h$ and $4h+2$, respectively.

The *inner dual ID* of a phenylene (and of its hexagonal squeeze) is a tree, the vertices of which correspond to the hexagons; two vertices are adjacent if the respective two hexagons are first neighbors (see Figure 18).

The following peculiar relation between the W-values of a phenylene, its hexagonal squeeze and its inner dual was first empirically detected ([66]) and eventually demonstrated to be a generally valid result ([63, 99]):

THEOREM 8.4. *Let PH be a phenylene containing h hexagons and let HS and ID be the hexagonal squeeze and inner dual corresponding to PH. Then their Wiener indices are related as*

$$W(PH) = \tfrac{9}{4}[W(HS) + 16W(ID) - (4h+1)(2h+1)].$$

For a related result, see [84].

It seems that there exists and analogous relations between the Szeged indices of *PH*, *HS* and *ID* ([63, 68]), but – so far – its form could not be established.

Concluding this section and this review, we wish to mention some closely related investigations. The Wiener index was also examined for other classes of polycyclic graphs: bipartite polycyclic plane graphs with faces of equal, but arbitrary sizes ([3, 42, 46]), graphs of polyphenyls ([55]), polycyclic chains consisting of pentagons ([3, 21, 22]), graphs of polymers and fullerenes ([1, 80, 87, 98, 116]). Several other, so-called Wiener-type topological indices were studied for hexagonal systems and other polycyclic graphs ([13, 54, 88, 121]).

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