# New Congruence Relations for the Wiener Index of Cata-Condensed Benzenoid Graphs

Andrey A. Dobrynin

Sobolev Institute of Mathematics, Russian Academy of Sciences, Siberian Branch, Novosibirsk 630090, Russia

Received July 1, 1997

The Wiener index ($W$) is a graph invariant defined as the sum of distances between all pairs of vertices in a graph. Necessary and sufficient conditions for $W$-values of cata-condensed benzenoid graphs to be congruent modulo 16 are established. As a corollary, a necessary condition for the coincidence of Wiener indices of benzenoid graphs is formulated in terms of simple structural parameters.

## INTRODUCTION

The Wiener index is a well-known graph distance invariant introduced 50 years ago.[1] It is defined as the half-sum of distances between all ordered pairs of vertices of the respective graph $H$,

$$W(H) = \frac{1}{2} \sum_{u,v \in V(H)} d(u,v)$$

where $d(u,v)$ is the number of edges in a shortest path connecting the vertices $u$ and $v$ in $H$. Mathematical properties and chemical applications of the Wiener index are outlined in numerous reviews and books.[2−14] In particular, some remarkable regularities of $W$ were discovered for graphs of cata-condensed benzenoid hydrocarbons. It was first demonstrated that the Wiener index of a cata-condensed benzenoid molecule must be an odd number.[15] Then it was shown that only every eighth number from the interval of possible values is available for $W$.[16,17] These properties were used for the estimation of the so-called mean isomer degeneracy of cata-condensed benzenoid hydrocarbons,[18−20] in searching for nonisomeric unbranched benzenoid hydrocarbons with equal $W$-values[21] and in other investigations.[22,23] New congruence relations have been recently established for unbranched cata-condensed benzenoid hydrocarbons with an equal number of rings.[24,25] For instance, it has been shown that the difference $W(H) - W(H')$ is divisible by 16 for any hexagonal chains $H$ and $H'$ under simple conditions.

In this paper we consider cata-condensed benzenoid graphs and derive necessary and sufficient conditions for their $W$-values to be congruent modulo 16. As a corollary, a necessary condition for the coincidence of Wiener indices is formulated in terms of simple structural characteristics.

## BENZENOID GRAPHS AND THEIR SEGMENTS

In this section we define a class of graphs which include molecular graphs of cata-condensed benzenoid hydrocarbons.[26] *Benzenoid graphs* are composed exclusively of six-membered cycles (hexagonal rings or hexagons). We assume that a graph contains at least two hexagons. Any two hexagons either have one common edge (and are then said to be adjacent) or have no common vertexes. No three hexagons share a common vertex. Each hexagon is adjacent to two or three other hexagons, with the exception of the *terminal hexagons* to which a single hexagon is adjacent. The *characteristic graph* of a given benzenoid graph consists of vertices corresponding to hexagons of the graph; two vertices are adjacent if and only if the corresponding hexagons share an edge.[27] A benzenoid graph is called *cata-condensed* if its characteristic graph is a tree. If all hexagons are regular, then the above defined graphs include nonplanar molecular graphs corresponding to helicenic benzenoid hydrocarbons.[26] The characteristic graph of a *hexagonal chain* is isomorphic to the simple path. An example of a cata-condensed benzenoid graph and its characteristic graph is shown in Figure 1a.

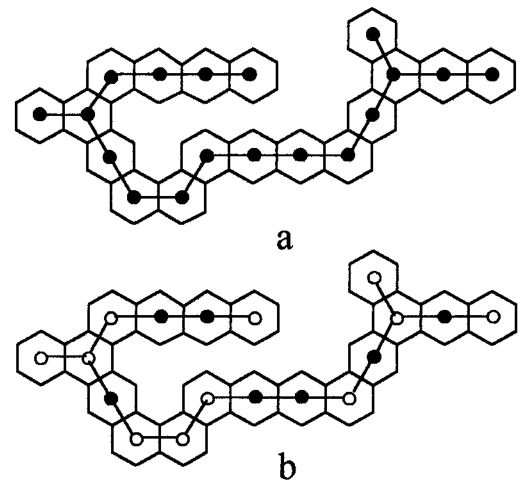

**Figure 1.** Characteristic graph and segments of benzenoid graph.

The set of all cata-condensed benzenoid graphs (or simply benzenoid graphs) with $h$ hexagons is denoted by $H_h$. It is easy to see that every graph $H$ from $H_h$ has $p_H = 4h + 2$ vertices and $q_H = 5h + 1$ edges.

Hexagons of a benzenoid graph may be angularly or linearly connected. Each angularly connected hexagon is said to correspond to a "kink" in the graph. As an illustration consider the graph shown in Figure 1b. White vertices of its characteristic graph correspond to angularly connected hexagons (pendent vertices are white for the convenience). Black vertices correspond to linearly connected hexagons.

S0095-2338(97)00047-4 CCC: $15.00 
Published on Web 03/06/1998

Let $H \in \mathcal{H}_h$ and $S \subseteq H$ be a hexagonal chain. Denote by $C_S$ a subgraph of the characteristic graph of $H$ induced by $S$. A subgraph $S$ is called the *segment* of $H$ if only pendent vertices of $C_S$ are white. Every segment shares a hexagon with its neighboring segment. The terminal segment has only one neighboring segment. The number of hexagons in a segment is called its length and is denoted by $l(S)$. It is clear that a segment is isomorphic to the linear polyacene and $2 \le l(S) \le h(H)$. We will assume that a benzenoid graph consists of a sequence of segments $S_1, S_2, ..., S_n$ with lengths $l(S_i) = l_i$. A segments' length of a graph forms an unordered family $\{l_1, l_2, ..., l_n\}$. For the graph in Figure 1, this family can be written as $\{4,2,2,3,2,2,4,3,2,3\} = \{2,2,2,2,2,3,3,3,4,4\}$. Let $n(H)$ be the number of all segments in a benzenoid graph $H$. Then $n(H) = n_o(H) + n_e(H)$, where $n_o(H)$ and $n_e(H)$ denote the numbers of segments with odd and even length, respectively.

## STATEMENT OF THE RESULT

A well-known result from the theory of the Wiener index states that $W(H) \equiv W(H')$ (*mod* 8) for benzenoid graphs $H$, $H' \in \mathcal{H}_h$; *i.e.*, the difference $W(H) - W(H')$ is divisible by 8.[16,17] Some conditions for the congruence relation $W(H) \equiv W(H')$ (*mod* 16) have been recently established for hexagonal chains of certain classes.[24,25] We now derive new necessary and sufficient conditions that provide the rule of modulo 16 for Wiener indices of benzenoid graphs.

**Theorem.** *Let $H$ and $H'$ be arbitrary cata-condensed benzenoid graphs in $\mathcal{H}_h$. Then $W(H) \equiv W(H')$ (mod 16) if and only if $n_e(H) \equiv n_e(H')$ (mod 4).*

The obtained result immediately leads to a necessary condition for the coincidence of $W$-values of benzenoid graphs.

**Corollary 1.** *Let $H$ and $H'$ be arbitrary cata-condensed benzenoid graphs in $\mathcal{H}_h$. If $W(H) = W(H')$, then $n_e(H) - n_e(H')$ is divisible by 4.*

The obtained congruence relation induces decomposition the set of benzenoid graphs $\mathcal{H}_h$ into four disjoint subsets $\mathcal{G}_0$, $\mathcal{G}_1$, $\mathcal{G}_2$, and $\mathcal{G}_3$ so that a graph of $\mathcal{G}_i$ contains $i + 4k$ ($k = 0,1,2...$) segments having even length. If benzenoid graphs $H$ and $H'$ belong to the distinct subsets, then $W(H) \neq W(H')$. It should be noted that segments of even length can be easily recognized in benzenoid graphs by hand.

## KINK TRANSFORMATIONS OF A GRAPH

Let us consider two graph operations of a benzenoid graph $H$ that consist in decomposing a terminal segment of $H$ into new segments $S_1$ and $S_2$ as shown in Figure 2 (the upper arrows). In other words, a terminal part of $S$ is displaced from its initial location to another one making new kinks in the resulting graph $H'$. Here and further, $A$ and $B$ stand for arbitrary fragments; in particular, they may be absent. An inverse operation fuses the segment $S_1$ and $S_2$ into the terminal segment $S$ (the lower arrows in Figure 2). These operations will be called the *kink transformations*. Every graph of $\mathcal{H}_h$ can be regarded as a result of kink transformations.

**Proposition 1.** *Let $H$ be an arbitrary cata-condensed benzenoid graph in $\mathcal{H}_h$. Then $H$ can always be obtained from the linear polyacene $L_h$ by a sequence of kink transformations.*

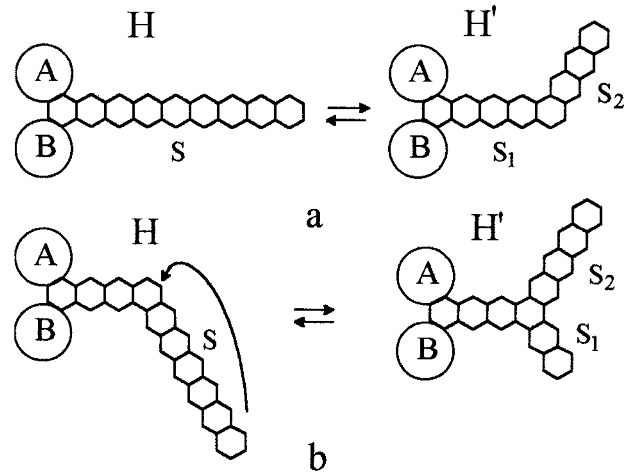


**Figure 2.** Kink transformation of a benzenoid graph.

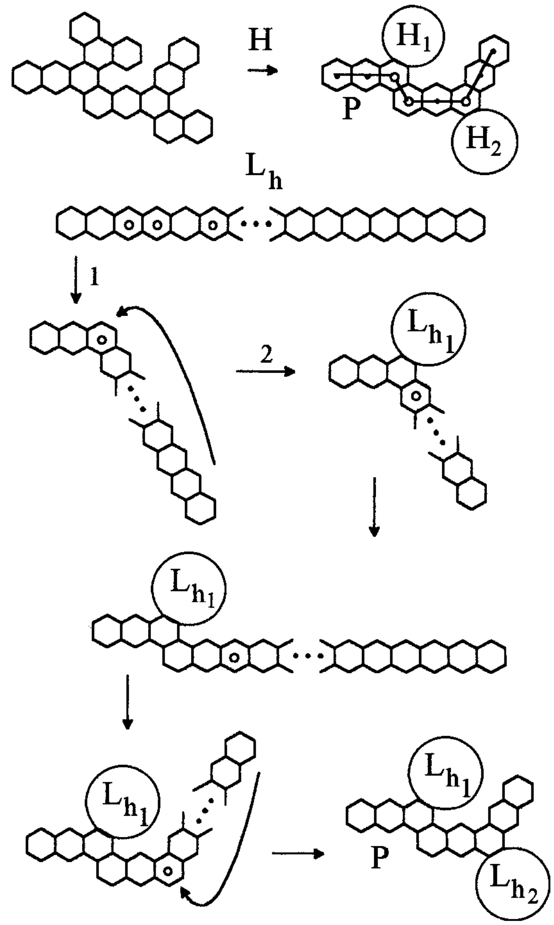


**Figure 3.** A sequence of transformations from $L_h$ to $H$.

**Proof.** Let $H \in \mathcal{H}_h$. We describe a simple constructive method to transform $L_h$ to $H$. This method is illustrated by graphs shown in Figure 3. First, choose an arbitrary hexagonal chain $P \subseteq H$ containing two terminal hexagons of $H$. Let $H_1, H_2, ..., H_k$ be subgraphs of $H$ attached to the chain $P$ (see Figure 3, $k = 2$). Consider the linear polyacene $L_h$ with $h = h_P + h_1 + h_2 + ... + h_k$ hexagons, where $h_i = h_{H_i}$. Then we begin to construct the chain $P$ from $L_h$ using kink transformations. It is obvious that the first possible transformation of $L_h$ is shown in Figure 2a (see also step 1 in Figure 3). Suppose that after several steps of this kind, a new kink in the resulting graph contains a hexagon such that

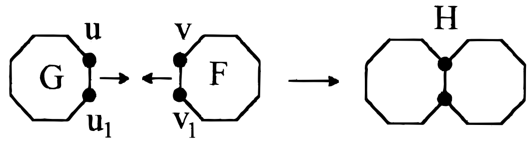


**Figure 4.**

the corresponding hexagon of $P$ connects with some $H_i$. Then we must cut the linear polyacene $L_{h_i}$ from the tail of the resulting graph and then join $L_{h_i}$ to this hexagon (see step 2). When the chain $P$ has been formed, we obtain the graph containing $P$ and the linear polyacenes $L_{h_1}$, $L_{h_2}$, ..., $L_{h_k}$ as shown in Figure 3 ($k = 2$). Next the above procedure is recursively applied to $L_{h_i}$ for all $i = 1, 2, ..., k$. It is easy to see that the resulting graph will be isomorphic to $H$.

**Corollary 2.** *Let H and H′ be arbitrary cata-condensed benzenoid graphs in $\mathcal{H}_h$. Then H′ can always be obtained from H by a sequence of kink transformations.*

**Proof.** Let $H, H' \in \mathcal{H}_h$. By Proposition 1, the graphs $H$ and $H'$ can be constructed from $L_h$ by kink transformations. Further, $L_h$ can be obtained from $H$ making use of inverse kink transformations. Therefore, the scheme of graph transformations $H \rightarrow L_h \rightarrow H'$ is always realized.

## CHANGES IN THE WIENER INDEX

In this section we study the changes in the Wiener index of benzenoid graphs under kink transformations. This allows one to determine what structural parameters of graphs are influenced by these changes.

By $D(v \mid H)$ we denote the *distance sum* of a vertex $v$: $D(v \mid H) = \sum_{u\in V(H)} d(u, v)$. For an arbitrary edge $e = (v, u)$ of a graph $H$, we define two disjoint vertex subsets $B_u(H) = \{w \mid d(w, u) < d(w, v)\}$ and $B_v(H) = \{w \mid d(w, v) < d(w, u)\}$. Let $b_u(H) = |B_u(H)|$ and $b_v(H) = |B_v(H)|$. It is easy to verify that $D(u \mid H) - D(v \mid H) = b_v(H) - b_u(H)$ for an arbitrary pair of adjacent vertices of a graph. It is a well-known fact that the distance sum of all vertices of a benzenoid graph are mutually congruent modulo 4.[16,17]

**Proposition 2.** *Let u,v be arbitrary vertices of an cata-condensed benzenoid graph H. Then the difference $D(u \mid H) - D(v \mid H)$ is divisible by 4.*

Let $G$ and $F$ be benzenoid graphs. Suppose that $H$ is obtained from these graphs by identifying the edges $(u, u_1) \in E(G)$ and $(v, v_1) \in E(F)$ as depicted in Figure 4. Then the Wiener index of the graph $H$ can be expressed using the indices of its subgraphs $G$ and $F$ as follows.[28,29]

**Proposition 3.** *For the graph H, we have*

$$W(H) = W(G) + W(F) + (p_G - 2)D(v \mid F) + (p_F - 2)D(u \mid G) + 2[b_{u1}(G) + b_{v1}(F) - b_{u1}(G)b_{v1}(F)] - (p_G + p_F) + 1 \quad (1)$$

Equation 1 provides the basis for the calculation of the change in the Wiener index produced by kink transformations. In order to compute $W$, we decompose graphs of Figure 2 into two subgraphs as shown in Figure 5. First consider the graphs shown in Figure 5a. Applying (1), we have

$$W(H) - W(H') = 2[b_{u2}(G) - b_{u1}(G)](b_v(H) - 1) \quad (2)$$

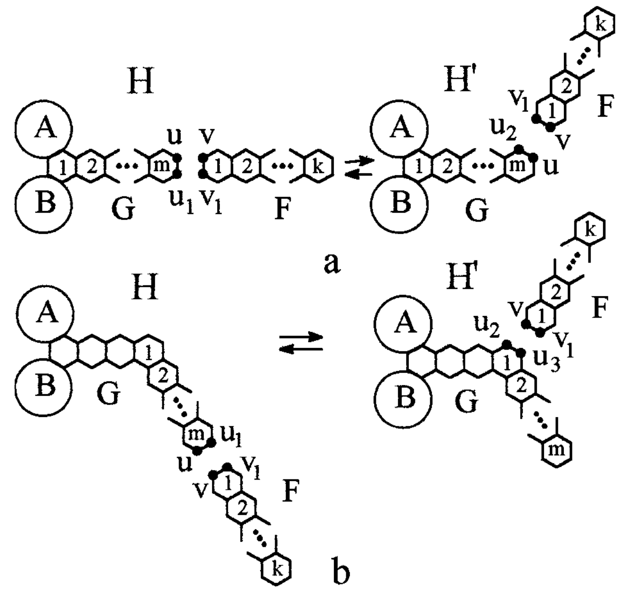


**Figure 5.** Graph decomposition for calculation of $W$.

It is easy to see that $b_{u_1}(G) = p_B + p_{L_m}/2 - 2 = p_B + 2m - 1$, $b_{u_2}(G) = p_A + p_B + (p_{L_m} - 3) - 4 = p_A + p_B + 4m - 5$, and $b_v(H) = p_{L_k}/2 = 2k + 1$. Substituting these terms back into (2), we arrive at

$$W(H) - W(H') = 16kh_A + 8k(m - 1) \quad (3)$$

Consider now the kink transformation depicted in Figure 5b. Then from eq 1,

$$W(H) - W(H') = 4h_F[D(u|G) - D(u_2|G)] + 2[b_{u3}(G) - b_{u1}(G)](b_v(H) - 1)$$

For this case, $b_{u_1}(G) = p_{L_m}/2 = 2m + 1$, $b_{u_3}(G) = p_{L_m} - 3 = 4m - 3$, and $b_v(H) = 2k + 1$. Then by taking into account Proposition 2, we can write the similar equation

$$W(H) - W(H') = 16k[2(m - 1)(h_G - m) + h_A - h_B] + 8k(m - 1) \quad (4)$$

Hence the difference $W(H) - W(H')$ is divisible by 16 if and only if the number $k(m + 1)$ is even. Note that $k = l(S_2) - 1$ and $m - 1 = l(S_1) - 1$. Therefore we have to examine the change of the parity of segments $S_1$,$S_2$, and $S$.

## CHANGE OF THE PARITY OF SEGMENTS

Let segments $S_1$ and $S_2$ be obtained from a terminal segment $S$ by a kink transformation. Here we denote this process as $S \leftrightarrow S_1S_2$. Then the change of the segments' parity will be denoted by the similar notation, for example, $E \leftrightarrow EO$. This means that $S$ has an even length and $S_1$ and $S_2$ have even and odd lengths, respectively. The following proposition can be proved by elementary observation.

**Proposition 4.** *The change of segments' parity under a kink transformation is described by one of the following cases: (a) $E \leftrightarrow EO$; (b) $E \leftrightarrow OE$; (c) $O \leftrightarrow OO$ and (d) $O \leftrightarrow EE$.*

Let $P = (l(S_1) - 1)(l(S_2) - 1)$.

**Corollary 3.** *Let $S \leftrightarrow S_1S_2$. Then the product P is always even for the cases (a)−(c) and always odd for the case (d).*

These facts lead to the following result.

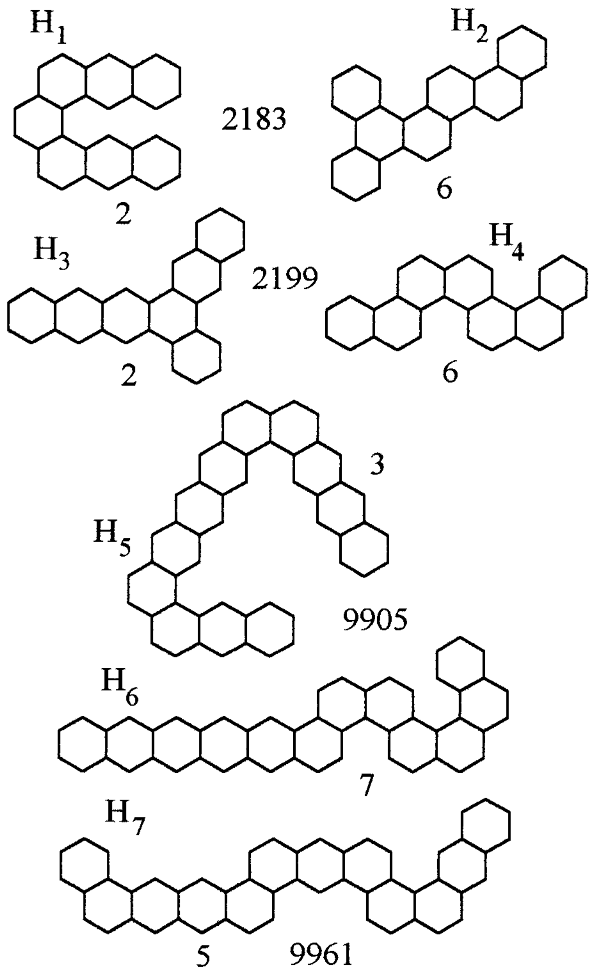


**Figure 6.** Some benzenoid graphs and numbers of their segments having even length.

**Proposition 5.** *Let $H$ and $H'$ be arbitrary cata-condensed benzenoid graphs in $\mathcal{H}_h$. Suppose that the case (d) occurs $N$ times under transferring from $H$ to $H'$. Then $W(H) \equiv W(H')$ (mod 16) if and only if $N$ is an even number.*

**Proof.** Because of Corollary 3, we need to examine only the case (d). Let us again consider eqs 3 and 4. Since $P$ is odd, it follows that $k = 2r + 1$ and $m - 1 = 2s + 1$ for some integers $r$ and $s$. Substituting these values into (3) and (4), we have

$$W(H) - W(H') = 16k[...] + 8(2r + 1)(2s + 1) = 16[...] + 8$$

This implies Proposition 5.

The last step of the proof of Theorem consists of counting the number of segments having even lengths.

## NUMBER OF SEGMENTS HAVING EVEN LENGTH

Let $H$ and $H'$ be arbitrary cata-condensed benzenoid graphs in $\mathcal{H}_h$, and $H'$ is obtained from $H$ by kink transformations. The following result shows how $n_e$ changes in the simplest case.

**Proposition 6.** *(i) Let a kink transformation be applied one time. Then $n_e(H') \in \{n_e(H) - 2, n_e(H), n_e(H) + 2\}$; (ii) the number of hexagons $h_H$ and $n_e(H)$ always have distinct parity.*

**Proof.** It suffices to note that the number of segments having even length does not change in the cases $E \leftrightarrow EO$, $E \leftrightarrow OE$, and $O \leftrightarrow OO$. However, this number increases by 2 in the case $O \rightarrow EE$ (decreases by 2 in the case $O \leftarrow EE$).

Let $H$ and $H'$ be obtained from the linear polyacene $L_h$, and the case (d) occurs $M$ and $M'$ times, respectively. Since $N = M + M'$ must be an even number, $M$ and $M'$ are both even or both odd.

Let $h$ be odd. If $M$ and $M'$ are even, then $n_e(H) = 2M = 4r$ and $n_e(H') = 2M' = 4s$ for some integers $r$ and $s$. If $M$ and $M'$ are odd, then $n_e(H) = 2M = 2(2r + 1) = 4r + 2$ and $n_e(H') = 2M' = 4s + 2$. Therefore, $n_e(H) - n_e(H') = 4(r - s)$ and $n_e(H) + n_e(H') = 4(r + s + 1)$.

Let $h$ be even. Since $L_h$ has even length, we must add 1 to the above values of $n_e(H)$ and $n_e(H')$.

The proof of Theorem is complete.

From the above considerations, the main results may be reformulated in the following manner.

**Corollary 4.** *Let $H$ and $H'$ be arbitrary cata-condensed benzenoid graphs in $\mathcal{H}_h$. Then $W(H) \equiv W(H')$ (mod 16) if and only if $n_e(H) + n_e(H')$ is divisible by 4 for odd $h$, and $n_e(H) + n_e(H') - 2$ is divisible by 4 for even $h$.*

**Corollary 5.** *Let $H$ and $H'$ be arbitrary cata-condensed benzenoid graphs in $\mathcal{H}_h$. If $W(H) = W(H')$, then $n_e(H) + n_e(H')$ is divisible by 4 for odd $h$ and $n_e(H) + n_e(H') - 2$ is divisible by 4 for even $h$.*

If $H$ and $H'$ have the same numbers of segments, then $n_e(H)$ may be replaced by $n_o(H)$. Namely, $W(H) \equiv W(H')$ (*mod* 16) if and only if $n_o(H) - n_o(H')$ is divisible by 4. This result has been recently established for hexagonal chains by a completely different way of reasoning.[24]

## ANOTHER CONGRUENCE RELATION

If graphs have segments with prescribes lengths, then the congruence relation may be strengthened. We show that the congruence modulo 32 is valid for some subclasses of benzenoid graphs.

**Proposition 7.** *Let $H, H' \in \mathcal{H}_h$ and $h$ is odd. If all segments of $H$ and $H'$ have odd length, then $W(H) \equiv W(H')$ (mod 32).*

**Proof.** The graph $H$ can be obtained from $H'$ by a sequence of transformations $O \leftrightarrow OO$. It is easy to see that the integers $k$ and $m - 1$ in eqs 3 and 4 must be even for this transformation. This immediately implies Proposition 7.

If $h$ is even, then every graph of $\mathcal{H}_h$ has at least one segment of even length. Let $\mathcal{G}_h \subset \mathcal{H}_h$ consists of graphs having a single segment with even length. Suppose that such a segment is terminal for every graph $H \in \mathcal{G}_h$ and denote its length by $l(H)$.

**Proposition 8.** *Let $H, H' \in \mathcal{G}_h$. Then $W(H) \equiv W(H')$ (mod 32) if and only if the difference $l(H) - l(H')$ is divisible by 4.*

**Proof.** By construction, the graphs $H$ and $H'$ can be obtained from the linear polyacene by a sequence of transformations: $E \rightarrow EO$, $O \rightarrow OO$, .... Then it is sufficient to examine the change of $W$ under the first transformation, $E \rightarrow EO$. Note that this transformation occurs two times in the scheme $H \rightarrow H'$. Let $H_1$ be obtained from $L_h$ so that a terminal segment has even length in $H_1$. It is clear that the integers $k$ and $m$ in eq 3 are even and $h_A = 0$. Then we have

$$W(L_h) - W(H_1) = 8(2r)(2s + 1) = 32rs + 16r$$

Therefore, $W(H) \equiv W(H')$ (*mod* 32) if and only if $r$ is even and $W(H) \equiv W(H')$ (*mod* 16), otherwise. Since $k = h - l(H)$, Proposition 8 follows by elementary calculation.

We can see that if $W(H) = W(H')$ then $l(H) \equiv l(H')$ (*mod* 4) for the terminal segments of graphs $H, H' \in G_h$.

## EXAMPLES

To illustrate the basic obtained relations, consider benzenoid graphs depicted in Figure 6. The numbers of segments with even length as well as their Wiener indices are shown near every graph. Pairs of graphs $H_1$, $H_2$ and $H_3$, $H_4$ have odd number of hexagons, $h = 7$; $W(H_1) = W(H_2) = 2183$ and $W(H_3) = W(H_4) = 2199$. Benzenoid chains $H_5$,$H_6$ , and $H_7$ have 12 hexagons; $W(H_5) = W(H_6) = 9905$ and $W(H_7) = 9961$. Pairs of graphs $H_1$, $H_3$ and $H_1$, $H_4$ confirm that the condition of Corollary 1 is only necessary for coincidence of $W$.

## ACKNOWLEDGMENT

The author would like to thank the referees for many helpful suggestions.

## REFERENCES AND NOTES

(1) Wiener, H. Structural determination of paraffin boiling points. *J. Am. Chem. Soc.* **1947**, *69*, 17−20.
(2) Trinajstić, N. *Chemical Graph Theory*; CRC Press: Boca Raton, FL, 1983; 2nd ed., 1992.
(3) Balaban, A. T.; Motoc, I.; Bonchev, D.; Mekenyan, O. Topological indices for structure−activity correlations. *Topics Curr. Chem.* **1983**, *114*, 21−55.
(4) Bonchev, D. *Information Theoretic Indices for Characterization of Chemical Structure*; Research Studies Press: Chichester, 1983.
(5) Gutman, I.; Polansky, O. E. *Mathematical Concepts in Organic Chemistry*; Springer-Verlag: Berlin, 1986.
(6) Gutman, I.; Yeh, Y. N.; Lee, S. L.; Luo, Y. L. Some recent results in the theory of the Wiener number. *Indian J. Chem.* **1993**, *32a*, 651−661.
(7) Rouvray, D. H. The topological matrix in quantum chemistry. In Balaban,A. T., Ed.; *Chemical Applications of Graph Theory*; Academic Press: London, 1975; pp 175−222.
(8) Rouvray, D. H. Should we have designs on topological indices? In King, R. B., Ed.; *Chemical Applications of Topology and Graph Theory*; Elsevier: Amsterdam, 1983; pp 159−177.
(9) Canfield, E. R.; Robinson, R. W.; Rouvray, D. H. Determination of the Wiener molecular branching index for the general tree. *J. Comput. Chem.* **1985**, *6*, 598−609.
(10) Rouvray, D. H. Predicting chemistry from topology. *Sci. Amer.* **1986**, *255*, 36−43.
(11) Rouvray, D. H. The modeling of chemical phenomena using topological indices. *J. Comput. Chem.* **1987**, *8*, 470−480.
(12) *Chemical Graph Theory. Introduction and Fundamentals*; Bonchev, D., Rouvray, D. H., Eds.; Gordon & Breach: Reading, U.K., 1991.
(13) Mihalić, Z.; Veljan, D.; Amić, D.; Nikolić, S.; Plavšić, D.; Trinajstić, N. The distance matrix in chemistry. *J. Math. Chem.* **1992**, *11*, 223−258.
(14) Nikolić, S.; Trinajstić, N.; Mihalić, Z. The Wiener index: developments and applications. *Croat. Chem. Acta* **1995**, *68*, 105−129.
(15) Bonchev, D.; Gutman, I.; Polansky, O. E. Parity of the distance and Wiener numbers of bipartite graphs. *Comm. Math. Comput. Chem. (MATCH)* **1987**, *22*, 209−214.
(16) Gutman, I. Wiener numbers of benzenoid hydrocarbons: two theorems. *Chem. Phys. Lett.* **1987**, *136*, 134−136.
(17) Gutman, I. On distances in some bipartite graphs. *Publ. Inst. Math. (Beograd)* **1988**, *43*, 3−8.
(18) Gutman, I.; Marković, S.; Luković, D.; Radivojević, V.; Rančić, S. On Wiener numbers of benzenoid hydrocarbons. *Coll. Sci. Papers Fac. Sci. Kragujevac* **1987**, *8*, 15−34.
(19) Dobrynin, A. A. Distribution of the distance number of unbranched hexagonal system graphs. *Vychisl. Sistemy* **1990**, *136*, 61−141, in Russian.
(20) Dobrynin, A. A. Graph distance numbers of nonbranched hexagonal systems. *Siberian Adv. Math.* **1992**, *2*, 121−134.
(21) Dobrynin, A. A. Graphs of unbranched hexagonal systems with equal values of the Wiener index and different number of rings. *J. Math. Chem.* **1992**, *9*, 239−252.
(22) Dobrynin, A. A.; Gutman, I. On the Szeged index of unbranched catacondensed benzenoid molecules. *Croat. Chem. Acta* **1996**, *69*, 845−856.
(23) Dobrynin, A. A. The Szeged index for complements of hexagonal chains. *Comm. Math. Comput. Chem. (MATCH)* **1997**, *35*, 227−242.
(24) Dobrynin, A. A. Congruence relations for the Wiener index of hexagonal chains. *J. Chem. Inf. Comput. Sci.*, in press.
(25) Dobrynin, A. A. A new formula for the calculation of the Wiener index of hexagonal chains. *Comm. Math. Comput. Chem. (MATCH)* **1997**, *35*, 75−90.
(26) Gutman, I.; Cyvin, S. J. *Introduction to the Theory of Benzenoid Hydrocarbons*; Springer-Verlag: Berlin, 1989.
(27) Balaban, A. T.; Harary, F. Chemical graphs. V. Enumeration and proposed nomenclature of benzenoid cata-condensed polycyclic aromatic hydrocarbons. *Tetrahedron* **1968**, *24*, 2505−2516.
(28) Polansky, O. E.; Bonchev, D. The Wiener number of graphs. I. General theory and changes due to some graph operations. *Comm. Math. Comp. Chem. (MATCH)* **1986**, *21*, 133−186.
(29) Polansky, O. E.; Bonchev, D. Theory of the Wiener number of graphs. II. Transfer graphs and some of their metric properties. *Comm. Math. Comput. Chem. (MATCH)* **1990**, *25*, 3−39.

CI970047C