GRAPHS OF UNBRANCHED HEXAGONAL SYSTEMS WITH EQUAL VALUES OF THE WIENER INDEX AND DIFFERENT NUMBERS OF RINGS

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Abstract

Graphs of unbranched hexagonal systems consist of hexagonal rings connected with each other. Molecular graphs of unbranched polycyclic aromatic hydrocarbons serve as an example of graphs of this class. The Wiener index (or the Wiener number) of a graph is defined as the sum of distances between all pairs of its vertices. Necessary conditions for the existence of graphs with different numbers of hexagonal rings and equal values of the Wiener index are formulated, and examples of such graphs are presented.

1. Introduction

One of the promising trends of mathematical chemistry is the construction and investigation of molecular graph invariants which could be used to describe structures of chemical compounds. Such invariants, called topological indices, are used to reveal molecular similarity, order isomers, and compare molecular skeleton forms, characterize molecular branching and cycling, establish the relationship between structure and properties of molecules, predict biological activity of chemical compounds, etc. [1-5]. Among a great number of papers on topological indices, two trends are discernible. The papers of the first trend are dedicated to the construction and application of topological indices to particular problems of chemistry. The papers of the second trend deal with the properties of topological indices as mathematical objects. There is a close relationship between the above trends as, on the one hand, a profound mathematical investigation covers the indices which have already shown their advantages in chemical applications and, on the other hand, the mathematical analysis of the index properties provides additional information to a scientist by revealing the features of the indices' behaviour and possible restrictions, thus allowing the use of the indices with a greater comprehension.

The most important characteristic of any topological index is its sensitivity in the process of molecular structure classification. If topological index values coincide for two different molecular graphs, i.e. the index degenerates on these structures, then it is less sensitive than the index which differentiates these graphs. In problems of compound property prediction, the assumption is often used that molecules with similar structures (or values of the index as a measure of similarity) have similar properties. Thus, the discriminating ability of the index and the structure of graphs where the index degenerates are important for the investigation of topological indices.

The Wiener index (or the Wiener number), which is equal to the sum of distances between all pairs of molecular graph vertices, is one of the most well-known topological indices. For this index and its modifications, the relationship is established between its values and properties of chemical compounds, in particular, polycyclic aromatic structures [6–11].

2. Basic definitions

We consider finite connected graphs without loops and multiple edges; $V(G)$ is a set of vertices of the graph G and $|V(G)|$ is the order of the graph. Define a class of graphs where all internal faces on a plane are hexagonal, and two arbitrary faces either have only a common edge (i.e. they are adjacent), or have no common vertices. Each face is adjacent to no more than two other faces. Hexagonal faces together with their bound are called the rings of the graph. By placing each hexagonal ring in correspondence with a new vertex and then joining them (if the corresponding rings are adjacent), we obtain the characteristic graph of the initial one. A set of graphs consisting of h rings for which their characteristic graph is isomorphic to a simple path is denoted by $\mathcal{G}_h$. Graphs G_1, G_2 and G_3 (see fig. 1) belong to the class $\mathcal{G}_h$.

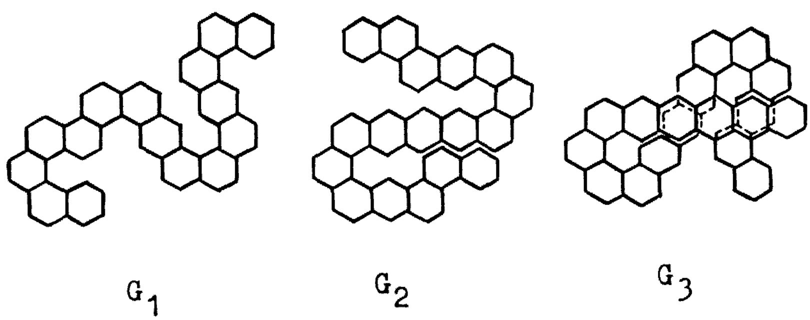


Fig. 1.

Graphs of this class model molecular structures of unbranched cata-condensed benzenoid hydrocarbons [12]. The order of any graph from $\mathcal{G}_h$ is obviously equal to $4h + 2$, and all vertices of the graph have degree 2 or 3. By the distance $d(u, v)$ between vertices v, $u \in V(G)$ we mean the length of a simple path which joins the vertices v and u in the graph G and contains the minimal number of edges. The Wiener index of the graph G is determined as $W(G) = \frac{1}{2}\sum_{v,\,u \in V(G)} d(v, u)$. The set of graphs $\mathcal{G}_h$ can be divided into two disjoint subsets $\mathcal{G}_h = \mathcal{L}_h \cup \mathcal{N}_h$, where the set $\mathcal{L}_h$ is composed of the graphs which are embedded into a regular hexagonal lattice on a plane (see graph G_1 in fig. 1), while graphs of the class $\mathcal{N}_h$ cannot be embedded into a hexagonal lattice (graphs G_2 and G_3 in fig. 1).

3. Properties of the unbranched hexagonal system graphs with equal Wiener index

In this section, we formulate the necessary conditions for the existence of graphs with equal values of the Wiener index and different numbers of rings. To continue, we need certain results from the theory of the Wiener index of hexagonal system graphs.

STATEMENT 1 [13–15]

(a) The Wiener index of the unbranched hexagonal system graphs is an odd number;

(b) the Wiener index of an arbitrary graph $G \in \mathcal{G}_h$ is within the range

$$W_{\min}(h) \le W(G) \le W_{\max}(h),$$

where $W_{\min}(h) = \frac{1}{3}(8h^3 + 72h^2 - 26h + 27)$ and $W_{\max}(h) = \frac{1}{3}(16h^3 + 36h^2 + 26h + 3)$, and equality is reached on graphs presented in fig. 2;

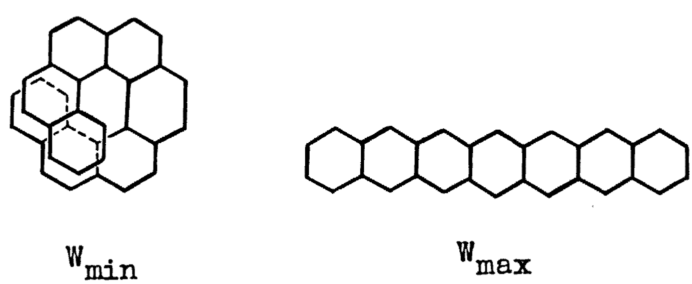


Fig. 2.

(c) $W(G_1) \equiv W(G_2) \pmod 8$ holds for the Wiener index value of two arbitrary graphs of hexagonal systems $G_1, G_2 \in \mathcal{G}_h$.

Define a set of possible values of the Wiener index for graphs of the class $\mathcal{G}_h$ as $E_h = \{W_{\min}(h) + 8n \mid n = 0, 1, \ldots, \frac{1}{8}(W_{\max}(h) - W_{\min}(h))\}$. The set E_h is a discrete interval of odd numbers of cardinality $|E_h| = \frac{1}{8}(W_{\max} - W_{\min}) + 1 = h(2h^2 - 9h + 13)$. Denote the set of the Wiener index values of all graphs of the class $\mathcal{G}_h$ as $W(\mathcal{G}_h)$, i.e. $W(\mathcal{G}_h) = \{W(G) | G \in \mathcal{G}_h\}$. The number $C(h)$ of graphs of the unbranched hexagonal systems with h rings is obtained as follows [16]:

$$C(h) = \begin{cases} \frac{1}{4}(3^{(h-2)/2} + 1)^2 & \text{for } h = 2, 4, 6, \ldots, \\ \frac{1}{4}(3^{h-2} + 3^{(h-1)/2} + 3^{(h-3)/2} + 1) & \text{for } h = 3, 5, 7, \ldots. \end{cases}$$

As the number of rings increases, the number of graphs of the class $\mathcal{G}_h$ increases in proportion to 3^h, while the number of possible values of the Wiener index increases only as h^3. Hence, the average cardinality of the index degeneration class (graphs with the same values of index) increases exponentially for each value of the index. Thus, the problem is naturally stated as the investigation of the Wiener index degeneration for graphs of $\mathcal{G}_h$, where the value of h is fixed. Such an investigation was pursued in [17–24], and the last paper presents complete information on the index degeneration classes in $\mathcal{G}_h$ for graphs with the number of rings $3 \le h \le 16$. The results of theoretical studies [17–19] and, particularly, [18,19], however, make it possible to construct large graphs with the same number of rings and equal values of the Wiener index quite easily. We consider the existence of graphs with a different number of rings and equal values of the Wiener index. In the present paper, the question "Are there graphs $G_1 \in \mathcal{G}_{h_1}$ and $G_2 \in \mathcal{G}_{h_2}$, $h_1 \ne h_2$, such that $W(G_1) = W(G_2)$?" is answered in the affirmative.

The obviously necessary condition for the existence of graphs with a different number of rings and equal values of the Wiener index is a non-empty intersection

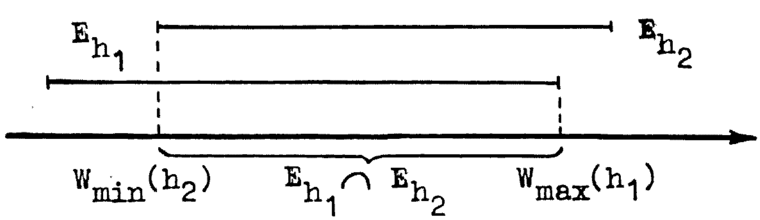


Fig. 3.

of the sets of the possible index values for graphs from classes $\mathcal{G}_{h_1}$ and $\mathcal{G}_{h_2}$, i.e. $E_{h_1} \cap E_{h_2} \ne \varnothing$ (see fig. 3). The condition for selecting the sets E_{h_1} and E_{h_2} establishes:

STATEMENT 2

If for graphs $G_1 \in \mathcal{G}_{h_1}$ and $G_2 \in \mathcal{G}_{h_2}$, $h_1 \ne h_2$, the values of the Wiener index coincide, $W(G_1) = W(G_2)$, then $h_1 \equiv h_2 \pmod 4$ holds for the number of rings of the graphs.

Proof

Let $h_1 < h_2$ and $h_2 = h_1 + k$. By virtue of the equality $W(G_1) = W(G_2)$ and the structure of the sets E_{h_1} and E_{h_2}, values $W_{\min}(h_2)$ and $W_{\min}(h_2 - k)$ are to be compatible by modulus 8. We have $W_{\min}(h_2) - W_{\min}(h_2 - k) = 8k(h_2 - k)(h_2 + 6) + \frac{2}{3}k(4k^2 + 36k - 1)$. The first term in the expression obtained is divisible by 8, and the value $4k^2 + 36k - 1$ is odd for any k. Therefore, the second term is divisible by 8, if and only if $k = 4m$, $m = 1, 2, 3, \ldots$. □

According to statement 2, graphs with equal values of the Wiener index cannot have a number of hexagonal rings which differs arbitrarily, i.e. such graphs should be sought for in the classes $\ldots \mathcal{G}_{h-8}, \mathcal{G}_{h-4}, \mathcal{G}_h, \mathcal{G}_{h+4}, \mathcal{G}_{h+8}, \ldots$ only. First consider the two nearest classes $\mathcal{G}_{h-4}$ and $\mathcal{G}_h$. The condition of the non-empty intersection of the sets E_{h-4} and E_h gives:

STATEMENT 3

If $h \geq 27$ holds for the number of rings in graphs from $\mathcal{G}_{h-4}$ and $\mathcal{G}_h$, then the set $E_{h-4} \cap E_h$ is non-empty.

Proof

The condition $E_{h-4} \cap E_h \neq \varnothing$ is equivalent to the inequality $W_{\max}(h-4) - W_{\min}(h) > 0$ being satisfied (see fig. 3). For the Wiener index difference, we have $W_{\max}(h-4) - W_{\min}(h) = \frac{1}{3}(8h^3 - 246h^2 + 532h - 576)$. The expression obtained takes on negative values for $3 \leq h \leq 26$, and positive values for $h \geq 27$. □

The information on the number of graphs in classes $\mathcal{G}_{h-4}$ and $\mathcal{G}_h$, the cardinality of the sets of the Wiener index values and their intersection is given in table 1 for certain values of h.

Since the Wiener index depends considerably on the number of vertices in graphs, so the number of rings in a graph from $\mathcal{G}_h$ is compensated for by shorter distances between its vertices than in a graph from the class $\mathcal{G}_{h-4}$. Thus, a graph from $\mathcal{G}_h$ is expected to be "similar" to a graph with the minimal value of the Wiener index in $\mathcal{G}_h$, while a graph from $\mathcal{G}_{h-4}$ is expected to be "similar" to a graph with the maximal value of the Wiener index in $\mathcal{G}_{h-4}$. If the cardinality of the set $E_{h-4} \cap E_h$ is low, then there will be no graphs with the Wiener index values belonging to $E_{h-4} \cap E_h$. As is shown in [24], the set $E_h \setminus W(\mathcal{G}_h)$ is non-empty for any $h > 3$. It can be presented as $E_h \setminus W(\mathcal{G}_h) = \cup_i [a_i, b_i]$, where $[a_i, b_i]$ are discrete intervals of values, some of which have cardinality proportional to h. The intervals are located in the starting and final parts of E_h, their cardinality decreasing from the bounds to the centre of E_h. Therefore, if the set $E_{h-4} \cap E_h$ is not sufficiently large, then it can be included in the set $(E_{h-4} \setminus W(\mathcal{G}_{h-4})) \cup (E_h \setminus W(\mathcal{G}_h))$; there exist no graphs which realize the elements of the latter. Pairs of graphs from classes $\mathcal{G}_{25}$

Table 1

Numbers of graphs in classes $\mathcal{G}_{h-4}$ and $\mathcal{G}_h$, the cardinality of the sets of Wiener index values and their intersection for several values of h.

$h-4$	h	$\lvert \mathcal{G}_{h-4} \rvert$	$\lvert \mathcal{G}_h \rvert$	$\lvert E_{h-4} \rvert$	$\lvert E_h \rvert$	$\lvert E_{h-4} \cap E_h \rvert$
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	2850
31	35	17157599124190	1389765184685602	8556	12530	3407

and $\mathcal{G}_{29}$ with equal values of the Wiener index are presented in fig. 4. For graphs G_1 and G_2, the index is $W(G_1) = W(G_2) = 89059$, and $W(G_3) = W(G_4) = 88035$ holds for graphs G_3 and G_4. For the intersection cardinality $|E_{25} \cap E_{29}| = 760$, the value $W(G_1)$ is the 511th value with respect to the left-hand side bound of the interval E_{29}, and the 250th value with respect to the right-hand side bound of E_{25}, while $W(G_3)$ is the 383rd value with respect to the left-hand side bound of E_{29} and the 378th value with respect to the right-hand side bound of E_{25}, i.e. $W(G_3)$ is almost in the centre of the interval $E_{25} \cap E_{29}$.

The above considerations deal with the whole set of graphs of the unbranched hexagonal systems $\mathcal{G}_h = \mathcal{L}_h \cup \mathcal{N}_h$. Extend similar reasoning individually to classes of graphs that can be embedded into a regular hexagonal lattice on a plane and those for which the embedding is not possible. Let us make use of the expression for extreme values of the Wiener index of graphs belonging to the above-mentioned classes.

STATEMENT 4 [24]

(a) The minimal value of the Wiener index for graphs from the class $\mathcal{L}_h$ is

$$W_{\min}(h) = \tfrac{1}{9}(32h^3 + 168h^2 + \varphi(h)),$$

where

$$\varphi(h) = \begin{cases} -6h+81, & \text{for } h = 3m, \quad m = 1,2,3,\dots, \\ -6h+49, & \text{for } h = 3m+1, \quad m = 0,1,2,\dots, \\ -54h+81, & \text{for } h = 3m+2, \quad m = 0,1,2,\dots . \end{cases}$$

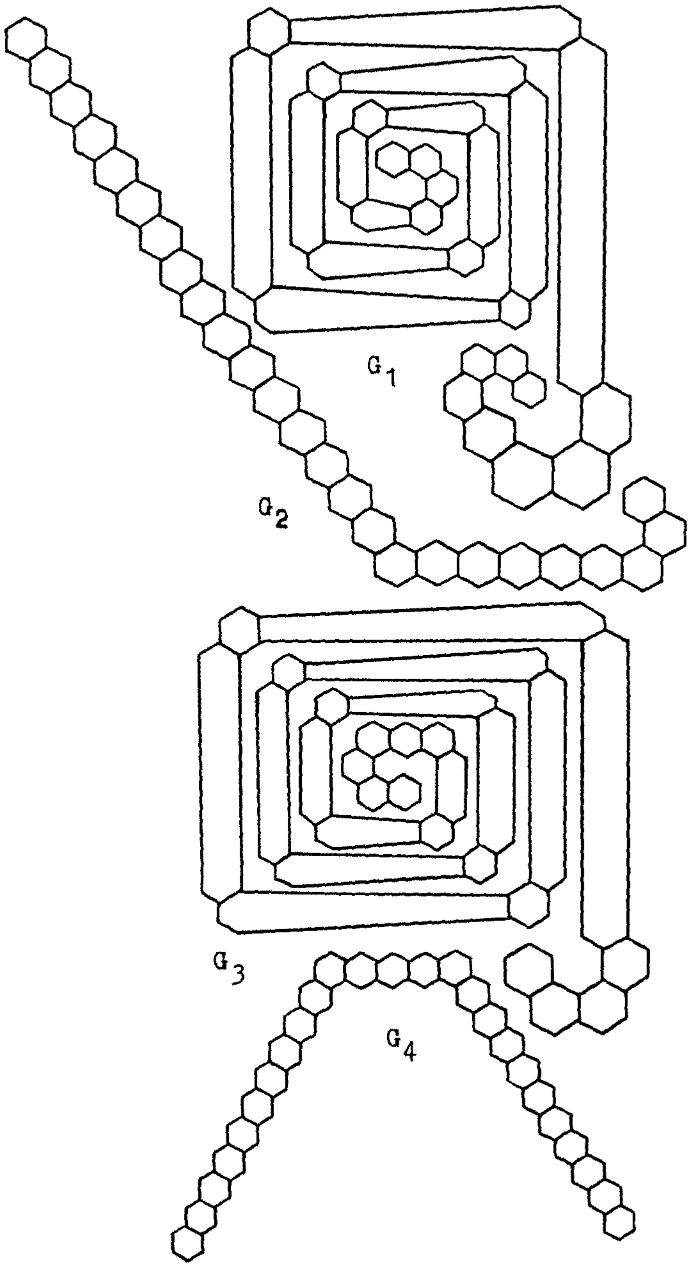


Fig. 4.

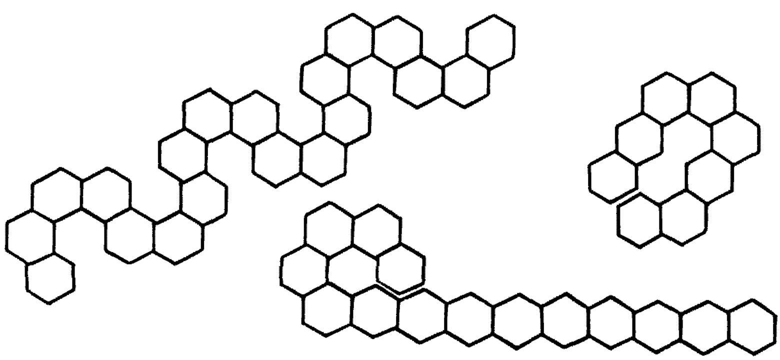
(b) The maximal value of the Wiener index for graphs from the class $\mathcal{N}_h$ is

$$W_{\max}(h) = \frac{1}{9}(16h^3 + 36h^2 - 358h + 1587) + \varphi(h),$$

where

$$\varphi(h) = \begin{cases} 8, & \text{for } h = 8, \\ 0, & \text{otherwise.} \end{cases}$$

Graphs for which the above values are reached are presented in fig. 5. The analysis of the intersections of the possible Wiener index values for $\mathcal{L}_h$ and $\mathcal{N}_h$ allows us to estimate the number of rings in graphs with equal values of the index.



W_{min} W_{max}

Fig. 5.

STATEMENT 5

If for graphs from the class $\mathcal{N}_h$ the number of rings is $h \geq 28$, and $h \geq 38$ holds for the number of rings of graphs from the class $\mathcal{L}_h$, then $E_{h-4} \cap E_h \neq \varnothing$.

The information on cardinalities of the Wiener index value intervals and their intersections for $\mathcal{N}_h$ and $\mathcal{L}_h$ is given in table 2. Let graphs G_1, G_3, $G_5 \in \mathcal{G}_{40}$ be obtained from the graph $H \in \mathcal{G}_{29}$ and the corresponding graphs with 11 rings as illustrated in fig. 6. Consider graphs G_2, G_4, $G_6 \in \mathcal{G}_{36}$ which are constructed analogously from the graph $H_1 \in \mathcal{G}_{21}$ and the corresponding pairs of graphs with 7 and 8 rings (see fig. 6). We have $G_1 \in \mathcal{L}_{40}$, $G_2 \in \mathcal{L}_{36}$ and $W(G_1) = W(G_2) = 262057$, $G_3 \in \mathcal{L}_{40}$, $G_4 \in \mathcal{N}_{36}$ and $W(G_3) = W(G_4) = 259033$, and $G_5 \in \mathcal{N}_{40}$, $G_6 \in \mathcal{N}_{36}$ and $W(G_5) = W(G_6)$ $= 258473$.

Table 2

Data for the classes $\mathcal{N}_h$ and $\mathcal{L}_h$.

Class	$h-4$	h	$\lvert E_{h-4}\rvert$	$\lvert E_h\rvert$	$\lvert E_{h-4}\cap E_h\rvert$
	24	28	3478	5820	149
	25	29	3991	6533	426
	26	30	4551	7301	742
	27	31	5160	8126	1099
$\mathcal{N}_h$	28	32	5820	9010	1499
	29	33	6533	9955	1944
	30	34	7301	10963	2436
	31	35	8126	12036	2977
	32	36	9010	13176	3569
	34	38	7811	11059	244
	35	39	8570	11960	549
	36	40	9330	12936	913
	37	41	10159	13989	1338
$\mathcal{L}_h$	38	42	11059	15043	1748
	39	43	11960	16178	2223
	40	44	12936	17396	2765
	41	45	13989	18615	3292
	42	46	15043	19921	3890

Thus, we have considered the necessary conditions for the existence of graphs with equal values of the Wiener index which belong to the nearest classes $\mathcal{G}_{h-4}$ and $\mathcal{G}_h$. Now we obtain conditions for the existence of a pair of graphs in classes $\mathcal{G}_{h_1}$ and G_{h_2} for arbitrary numbers h_1 and h_2, $h_1 < h_2$ and $h_1 \equiv h_2 \pmod 4$. Denote h_2 by h for convenience, and let $k = \frac{1}{4}(h - h_1)$. Then, the determination of the non-emptiness of the set $E_{h-4k} \cap E_h$ evidently reduces to the question whether the inequality $W_{\max}(h-4k) - W_{\min}(h) = \frac{4}{3}[2h^3 - 3h^2(16k+3) + h(192k^2 - 72k + 13) - 2k(128k^2 - 2k + 13) - 6] > 0$ holds. If we equate this expression to zero, then for any $k \geq 1$ the equation obtained (as a cubic polynomial in h) will have only one real root for $h > 0$. For graphs of the classes $\mathcal{L}_h$ and $\mathcal{N}_h$, it is necessary to take the corresponding values of maximal and minimal values of the Wiener index (for $\mathcal{L}_h$, we took $\varphi(h) = -54h + 81$). As a result, the number of rings h in graphs can be estimated through k which characterizes the difference in the number of rings for a pair of graphs.

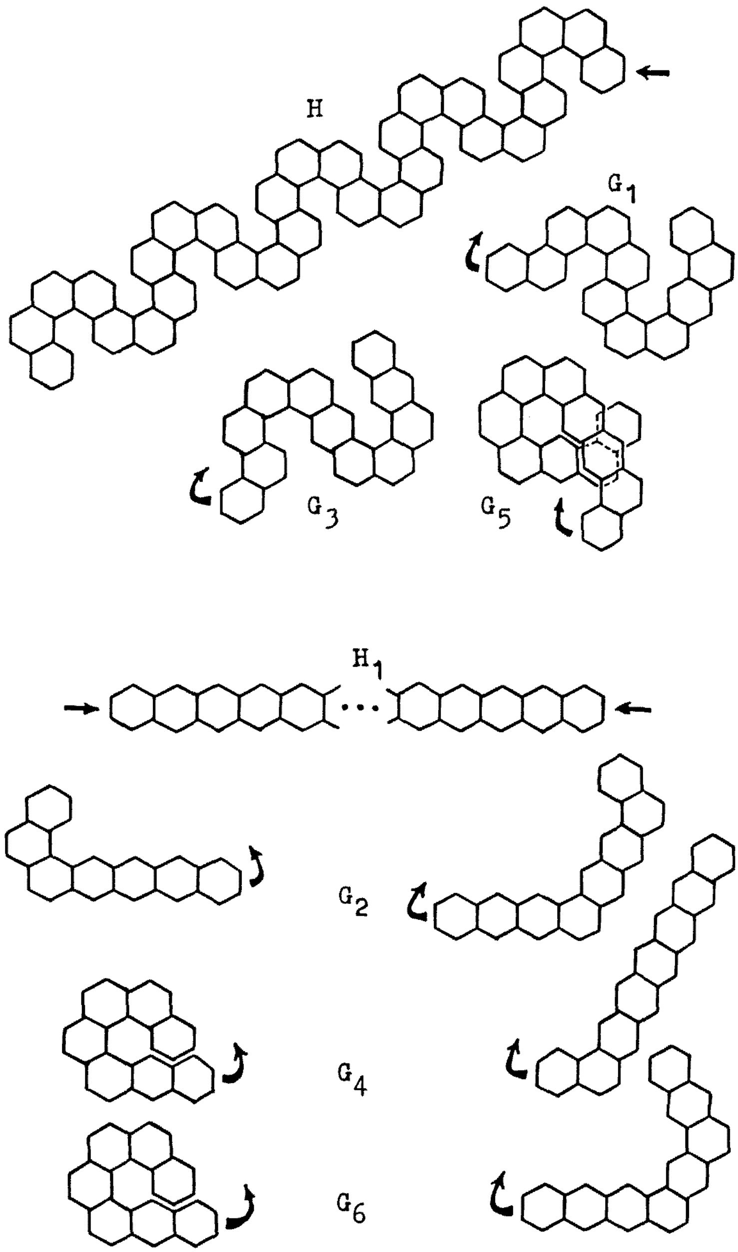


Fig. 6.

Table 3

Data for classes $\mathcal{G}_h$, $\mathcal{N}_h$ and $\mathcal{L}_h$, for $k=2$ and $k=3$.

Class	k	$h-4k$	h	$\|E_{h-4k}\|$	$\|E_h\|$	$\|E_{h-4k} \cap E_h\|$
$\mathcal{G}_h$	2	38	46	16207	29371	45
		39	47	17576	31396	686
		40	48	19020	33512	1386
		41	49	20541	35721	2147
		42	50	22141	38025	2971
		43	51	83822	40426	3860
		44	52	25586	42926	4816
		45	53	27435	45527	5841
		46	54	29371	48231	6937
	3	54	66	48231	89441	580
		55	67	51040	93666	1865
		56	68	53956	98022	3233
		57	69	56981	102511	4686
		58	70	60117	107135	6226
		59	71	63366	111896	7855
		60	72	66730	116796	9575
		61	73	70211	121837	11388
		62	74	73811	127021	13296
$\mathcal{N}_h$	2	39	47	17018	30710	128
		40	48	18446	32810	812
		41	49	19951	35003	1557
		42	50	21535	37291	2365
		43	51	23200	39676	3238
		44	52	24948	42160	4178
		45	53	26781	44745	5187
		46	54	28701	47433	6267
		47	55	30710	50226	7420
	3	55	67	50226	92660	1051
		56	68	53126	97000	2403
		57	69	56135	101473	3840
		58	70	59255	106081	5364
		59	71	62448	110826	6977
		60	72	65836	115710	8681
		61	73	69301	120735	10478
		62	74	72885	125903	12370
		63	75	76590	131216	14359

. . . continued

Table 3 (continued)

Class	k	$h-4k$	h	$\lvert E_{h-4k} \rvert$	$\lvert E_h \rvert$	$\lvert E_{h-4k} \cap E_h \rvert$
		62	70	49871	72221	847
		63	71	52332	75464	1938
		64	72	54916	78708	2998
		65	73	57625	82093	4167
	2	66	74	60335	85621	5447
		67	75	63174	89150	6696
		68	76	66144	92826	8060
		69	77	69115	96651	9541
		70	78	72221	100477	10991
$\mathcal{L}_h$						
		89	101	150221	220639	318
		90	102	155355	227273	2332
		91	103	160666	234108	4499
		92	104	166156	241146	6821
	3	93	105	171647	248185	9096
		94	106	177321	255431	11530
		95	107	183180	262886	14125
		96	108	189040	270342	16673
		97	109	195089	278011	19386

STATEMENT 6

If the number of rings in graphs from classes $\mathcal{G}_h$ and $\mathcal{N}_h$ satisfies the inequality $h \geq (k+1)n(k)$, and $h \geq (k+1)n_1(k)$ holds for the number of rings in graphs from the class $\mathcal{L}_h$, then $E_{h-4k} \cap E_h \neq \varnothing$, where

$$n(k) = \begin{cases} 14, & k=1, \\ 16, & k=2, \\ 17, & k=3, \\ 18, & 4 \leq k \leq 7, \\ 19, & 8 \leq k \leq 28, \\ 20, & k \geq 29, \end{cases} \quad \text{and } n_1(k) = \begin{cases} 19, & k=1, \\ 24, & k=2, \\ 26, & k=3, \\ 27, & k=4, \\ 28, & k=5,6, \\ 29, & k=7,8, \\ 30, & 9 \leq k \leq 14, \\ 31, & 15 \leq k \leq 38, \\ 32, & k \geq 39. \end{cases}$$

The minimal values of the number of rings in the inequalities from statement 6 exceed the minimal number of rings possible for graphs with such a property. The exact values of h for $k = 2$ (in a pair of graphs for which the number of rings differ by 8) and for $k = 3$ (the difference is 12) are given in table 3.

Consider necessary conditions for the existence of graphs with equal values of the Wiener index and several classes of graphs of the unbranched hexagonal systems with a different number of rings. Suppose there is a family of graphs $G_i \in \mathcal{G}_{h_i}$, $i = 1, 2, \ldots, m$, where $h_1 < h_2 < \ldots < h_m$ and $h_i \equiv h_j \pmod 4$ for all $i, j = 1, 2, \ldots, m$. The Wiener index will be the same in graphs $W(G_i) = W(G_j)$, $i, j = 1, 2, \ldots, m$ if the condition $\cap_{i=1}^{m} E_{h_i} \neq \emptyset$ is satisfied. It is easy to see that the equality $\cap_{i=1}^{m} E_{h_i} = E_{h_1} \cap E_{h_m}$ holds, i.e. the problem reduces to the case which has already been discussed, namely, the one where the index is the same for a pair of graphs. As the functions $W_{\min}(h)$ and $W_{\max}(h)$ increase monotonously with the increase of the number of rings h, $h \geq 1$, so $W_{\min}(h_i) \leq W(G) \leq W_{\max}(h_j)$ for any values $h_1 < h_j < h_i < h_m$, $i, j = 1, 2, \ldots, m$, if the inequality $W_{\min}(h_m) \leq W(G) \leq W_{\max}(h_1)$ holds. The number of rings of graphs with equal values of the Wiener index is given in table 3 for $k = 2$ (the case where the Wiener index is the same for three graphs) and for $k = 3$ (the index is the same for four graphs).

4. Conclusions

We consider simple necessary conditions for the existence of graphs of the unbranched hexagonal systems with a different number of rings and equal values of the Wiener index. We considered also the graphs which are embedded into a regular hexagonal lattice on a plane and the graphs for which the embedding is not possible. Examples of such graphs with the number of rings equal to 25 and 29, 36 and 40 are given. To obtain the graphs, we used the algorithms of fast generation of graphs of the unbranched hexagonal systems and those of the Wiener index calculation [25].

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