On the hyper Wiener index of hexagonal chains

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The hyper Wiener index of a molecular graph is defined as one half of the sum of the distances and the square distances between all (unordered) pairs of vertices of the graph. In this paper computation of the hyper Wiener index of some extremal hexagonal chains are purposed.

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1. Introduction

A real number that describes a molecular graph is called a topological index. Topological indices are one of the descriptors of molecules that play an important role in structure property and structure activity studies, particularly when multivariate regression analysis, artificial neural networks, and pattern recognition are used as statistical tools. The hyper Wiener index is one of the recently conceived distance-based graph invariants, used as a structure-descriptor for predicting physico–chemical properties of organic compounds (often those significant for pharmacology, agriculture, environment-protection etc.). The hyper Wiener index *WW(G)* of a graph *G* was proposed by Randic et al [1], as the generalization of the much studied Wiener index *W (G)* of graph invariant [2]. Recall that *W (G)* is defined as the sum of [3] distances between pairs of vertices of the graph. Let *G* be a simple connected graph. The sets of vertices and edges of G are denoted by *V (G)* and *E (G)*, respectively. For vertices *u* and *v* in *V (G),* we denote by *d (u, v)* the topological distance i.e., the number of edges on the shortest path, joining the two vertices of *G*. The hyper Wiener index of G is defined as follows:

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (d(u,v) + d^2(u,v)). \qquad (1)$$

A hexagonal system is a connected geometric figure obtained by arranging congruent regular hexagons. 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 are considerable importance in theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbon [4-7].

A hexagonal chain is a hexagonal system with the properties that (a) no vertex is incident with three hexagons, and (b) no hexagon is adjacent to more than two hexagons. Suppose that *H* is a hexagonal system. Denote by H_c the graph whose vertex set is the set of the centers of hexagons in *H*, and edge set of lines connecting the centers of any two adjacent hexagons. A hexagonal system *H* is a hexagonal chain if the graph H_c is a path. In this paper we consider both planar and non-planar (helicenic) hexagonal chains. This means that H_c may be a helix. Hexagonal chains are the graph representation of an important subclass of benzenoid molecules, unbranched catacondensed benzenoids molecules, which play a distinguished role in the theoretical chemistry of benzenoid hydrocarbons.

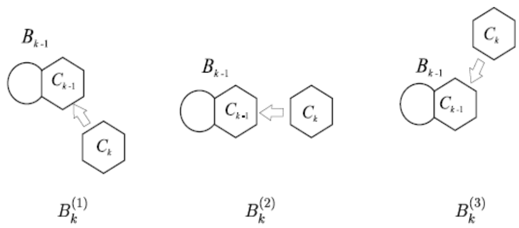

Fig. 1.

The extremal graphs with respect to some useful topological indices such as Wiener index in chemical applications have been extensively studies, any many results concerning this topic can be found in [8-10].

We write $B_n = C_1 C_2 ... C_n$ if $C_1, C_2, ..., C_n$ are the n hexagons of B_n, where C_i and C_{i+1} are adjacent for $i=1,2,..., n-1$. A hexagonal chain B_n, where $n>2$, can be obtained from a hexagon by a stepwise addition of terminal hexagons. At each step $k=2,3,..., n$, a type of addition is selected from the three possible constructions $B_{k-1} \rightarrow B_k^i = B_k$, *for i=1,2 or 3*, as depicts in *Fig 2*. We shall call the three possible constructions type I, type II and type III, respectively.

A hexagonal chain B_n is called *linear hexagonal chain*, denoted by L_n, if each mode of attachment of the hexagons is realized with type II construction (see Fig. 2). A hexagonal chain B_n is *fully angular* if each mode of attachment of the hexagons is realized with either type I construction or a type III construction. A fully angular hexagonal chain with n hexagons is called *zig-zag hexagonal chain*, denoted by Z_n, if each mode of attachment of the hexagons is realized alternated with a type I construction and a type III construction (see Fig. 3). It is called *helicene hexagonal chain*, denoted by H_n if all mode of attachment of the hexagons is realized with type I, or symmetrically, type III constructions (see Fig. 4). A fully angular hexagonal chain with n hexagons is called serpent hexagonal chain, denoted by S_n, if each mode of attachment of the hexagons is realized alternated with three type I construction and three type III construction (see Fig. 4). In this paper we compute the hyper Wiener index of L_n, Z_n and H_n in term of whose length of the hexagonal chain.

2. Results and discussion

In this section we will obtain exact formulas for the hyper Wiener index of L_n, Z_n and H_n in term of n, the length of these hexagonal chains. For this purpose sum of the distances between an arbitrary vertex of these hexagonal chains and other vertices of the graph must be computed. At first we consider the linear hexagonal chain. Among hexagonal chins with fixed number of hexagon, L_n has maximum Wiener index [13] and consequently hyper Wiener index.

Theorem 1. The hyper Wiener index of the linear hexagonal chain is computed as follows:

$$WW(L_n) = \frac{1}{3}(8n^4 + 32n^3 + 46n^2 + 37n + 3).$$

Proof: Let v_1 and v_2 be two adjacent vertices on i-th hexagon cycle of L_n. Symmetry of the graph shows that the vertices of L_n can be considered in two different types such as v_1 or v_2 on the first row or on the second row of the graph. It is because that sum of the distances between v_1 or v_2 and other vertices of the graph can be computed by two different methods. So it suffices that we compute sum of the distances between v_1 or v_2 and all of the other vertices of L_n. For this purpose we will calculate the distances between v_1 (or v_2) and the vertices on the first and second row of L_n where located before and after of v_1 (or v_2) separately.

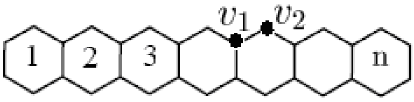

Fig 2. The graph of linear hexagonal chain.

A simple computation shows that sum of the distances and the square distances between v_1 and vertices on the first row of L_n is equal to

$$\sum_{j=1}^{2i-2}(j+j^2) + \sum_{j=1}^{2(h-i)+2}(j+j^2).$$

Also sum of the distances and the square distances between v_1 and vertices on the second row of L_n is equal to

$$\sum_{j=1}^{2i-1}(j+j^2) + \sum_{j=2}^{2(h-i)+3}(j+j^2).$$

If $d_1(i)$ denotes sum of the distances and the square distances between v_1 and other vertices of L_n, then

$$d_1(i) = \sum_{j=1}^{2i-2}(j+j^2) + \sum_{j=1}^{2(h-i)+2}(j+j^2) + \sum_{j=1}^{2i-1}(j+j^2) + \sum_{j=2}^{2(h-i)+3}(j+j^2).$$

Now let $d_2(i)$ denote sum of the distances and the square distances between v_2 and other vertices of L_n. Similar argument shows that

$$d_2(i) = \sum_{j=1}^{2i-1}(j+j^2) + \sum_{j=1}^{2(h-i)+1}(j+j^2) + \sum_{j=1}^{2i}(j+j^2) + \sum_{j=2}^{2(h-i)+2}(j+j^2).$$

Thus the hyper Wiener index of L_n can be computed by using $d_1(i)$, $d_2(i)$ and (1) as follows:

$$WW(L_n) = \frac{1}{2}\left(\sum_{i=1}^{n+1} d_1(i) + \sum_{i=1}^{n} d_2(i)\right) = \frac{1}{3}(8n^4 + 32n^3 + 46n^2 + 37n + 3).$$

Therefore the proof is completed.

In continue we will compute the hyper Wiener index of zig-zag hexagonal chain by using the exact formula of the Wiener index of Z_n where had been obtained by dobrynin et al [9]. Among hexagonal chains where each mode of attachment of the hexagons is realized with type I construction and type III construction (zig-zag construction) Z_n has minimum Wiener [9] and consequently hype Wiener index.

Theorem 2. The hyper Wiener index of zig-zag hexagonal chain is given as follows:

$$WW(Z_n) = \frac{1}{3}(8n^4 + 24n^3 + 28n^2 + 147n - 81).$$

Proof: Let C_i denote the i-th hexagon cycle of Z_n. We consider four vertices v_1, v_2, v_3, v_4 on C_i (see Fig. 3) and obtain a formula to computation sum of the square distances for these vertices. If $d_j(i)$ denotes sum of the square distances between v_j and other vertices of Z_n for $j=1,2,3,4$, by similar computation where had been used in Theorem *1* we have

$$d_1(i)=\sum_{j=1}^{2i-2} j^2+\sum_{j=1}^{2(h-i)+2} j^2+\sum_{j=1}^{2i-1} j^2+\sum_{j=2}^{2(h-i)+1} j.$$

$$d_2(i)=\sum_{j=1}^{2i-2} j^2+\sum_{j=1}^{2(h-i)+2} j^2+\sum_{j=3}^{2i-1} j^2+\sum_{j=4}^{2(h-i)+1} j+79.$$

$$d_3(i)=\sum_{j=1}^{2i-1} j^2+\sum_{j=1}^{2(h-i)+1} j^2+\sum_{j=4}^{2i} j^2+\sum_{j=3}^{2(h-i)} j+13$$

$$d_4(i)=\sum_{j=1}^{2i-1} j^2+\sum_{j=1}^{2(h-i)+1} j^2+\sum_{j=1}^{2i} j^2+\sum_{j=1}^{2(h-i)} j+13.$$

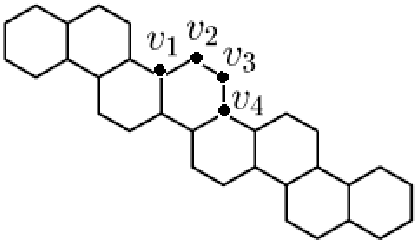

Fig. 3. The graph of zig-zag hexagonal chain.

On the other hand the wiener index of Z_n is computed as follows:

$$W(Z_n)=\frac{1}{3}(16n^3+24n^2+62n-21).$$

So the hyper Wiener index of L_n can be computed by using $d_j(i)$ for $j=1,2,3,4$ and *(1)* as follows:

$$WW(Z_n)=\frac{1}{2}\sum_{\{u,v\}\subseteq V}(d(u,v)+d(u,v)^2)$$
$$=\frac{1}{2}\sum_{i=1}^{n}(d_1(i)+d_4(i)+40)$$
$$+\frac{1}{2}\sum_{i=1}^{n}(d_2(i)+d_{34}(i)+128))$$
$$=\frac{1}{3}(8\mathrm{n}^4+24\mathrm{n}^3+28\mathrm{n}^2+147\mathrm{n}-81).$$

Therefore the proof is completed.

In the following Theorem the hyper Wiener index of helicene hexagonal chains will be computed. Among Fibonacenes with fixed number of hexagonal H_n has minimal Wiener [9] and consequently hyper Wiener index.

Theorem 3. The hyper Wiener index of helicene hexagonal chain is computed as follows:

$$WW(H_n)=\frac{1}{3}(2\mathrm{n}^4+28\mathrm{n}^3+154\mathrm{n}^2-169\mathrm{n}+111).$$

Proof: Let C_i denote the *i*-th hexagon cycle of H_n. Similar to Z_n we consider four vertices on C_i where are labeled by v_1, v_2, v_3, v_4 (see Fig. 4). If $d_j(i)$ denotes sum of the square distances between v_i and other vertices of H_n we have

$$d_1(i)=\sum_{j=2}^{i}(j^2+(j+1)^2+(j+2)^2+(j+3)^2)+$$
$$\sum_{j=2}^{h-i+1}(j^2+2(j+1)^2+(j+2)^2)+(i+1)^2+(i+2)^2-14.$$

$$d_2(i)=\sum_{j=3}^{i}(j^2+(j+1)^2+(j+2)^2+(j+3)^2)+$$
$$\sum_{j=4}^{h-i+3}(j^2+2(j+1)^2+(j+2)^2)+(i+1)^2+(i+2)^2-14.$$

$$d_3(i)=\sum_{j=4}^{i}(j^2+(j+1)^2+(j+2)^2+(j+3)^2)+$$
$$\sum_{j=4}^{h-i+2}(j^2+2(j+1)^2+(j+2)^2)+(i+2)^2+(i+3)^2+81.$$

$$d_4(i)=\sum_{j=0}^{i-1}(j^2+(j+1)^2+(j+2)^2+(j+3)^2)+$$
$$\sum_{j=1}^{h-i}(j^2+2(j+1)^2+(j+2)^2)+i^2+(i+1)^2.$$

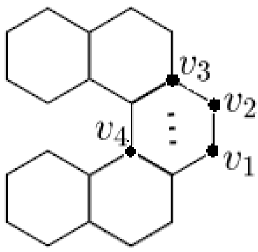

Fig. 4. The graph of helicene hexagonal chain.

Since $W(H_n)=\frac{1}{3}(8n^3+72n^2-26n+27)$ so the hyper Wiener index of H_n can be computed by using $d_j(i)$ for $j=1,2,3,4$ and *(1)* as follows

$$WW(H_n) = \frac{1}{2}\sum_{\{u,v\}\subseteq V}(d(u,v) + d(u,v)^2)$$

$$= \frac{1}{2}(\sum_{i=1}^{n}(d_1(i) + d_4(i) + 40)$$

$$+\sum_{i=1}^{n}(d_2(i) + d_{34}(i) + 128))$$

$$= \frac{1}{3}(8n^4 + 24n^3 + 28n^2 + 147n - 81).$$

Therefore the proof is completed.

At least we will compute the hyper Wiener index of serpent hexagonal chains. Among simple hexagonal chains with fixed number of hexagonal S_n has minimal Wiener [9] and consequently hyper Wiener index.

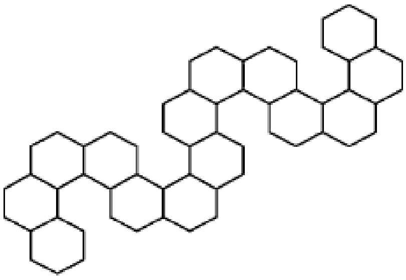

Fig. 5. The graph of serpent hexagonal chain.

Theorem 3. The hyper Wiener index of serpent hexagonal chain is computed as follows:

$$WW(S_n) = \frac{1}{27}(64n^4 + 448n^3 + \alpha).$$

Where α is given as

$$\alpha = \begin{cases} 1296n^2 - 1224n + 1755 & if \quad n = 3k \\ 1296n^2 - 1384n + 1115 & if \quad n = 3k+1. \\ 1104n^2 - 1976n + 3595 & if \quad n = 3k+2. \end{cases}$$

Proof: The results can be obtained by using similar argument of Theorem *2* and *3*.

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