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Two Topological Indices of Three Chemical Structures

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Abstract

In this paper, we present explicit formulas for computing the first and second vertex-edge Wiener indices of three classes of molecular graphs made by hexagons.

Introduction

Hexagonal systems are geometric objects obtained by arranging mutually congruent regular hexagons in the plane. They are of considerable importance in theoretical Chemistry, because they are natural graph representation of benzenoid hydrocarbons [1]. Each vertex in hexagonal system is either of degree two or three. Vertex shared by three hexagons is called an internal vertex of the respective hexagonal system. We call hexagonal system catacondensed if it does not possess internal vertices, otherwise we call it pericondensed.

A hexagonal chain is a catacondensed hexagonal system in which every hexagon is adjacent to at most two hexagons. Linear hexagonal chain is a hexagonal chain which is a graph representation of linear polyacene. When a linear hexagonal chain is bent so that its ends meet, a cyclic linear hexagonal chain is produced. A linear hexagonal chain and a cyclic linear

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hexagonal chain with n hexagons will be denoted by L_n and T_n, respectively. See Fig. 1 and Fig. 2.

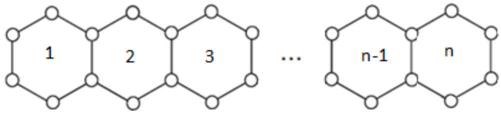

Fig. 1 Linear hexagonal chain L_n .

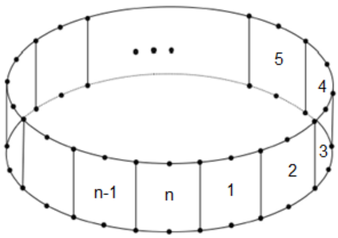

Fig. 2 Cyclic linear hexagonal chain T_n .

Double hexagonal chain is a chain consisted of two condensed identical hexagonal chains. It can be considered as benzenoid constructed by successive fusions of successive naphthalenes along a zig-zag sequence of triples of edges as appear on opposite sides of each naphthalene unit. Double linear hexagonal chain is consisted of two condensed linear hexagonal chains. Such chain will be denoted by B_{2n}, where n is the number of hexagons in the corresponding linear hexagonal chain. See Fig. 3.

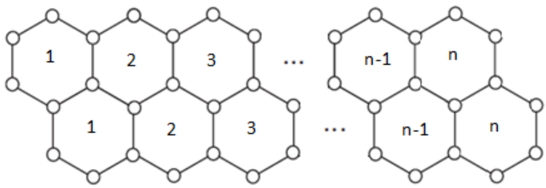

Fig. 3 Double linear hexagonal chain B_{2n} .

In theoretical Chemistry, the physico-chemical properties of chemical compounds are often modeled by the molecular graph based molecular structure descriptors which are also referred to as topological indices [2]. Among the variety of those indices, which are designed to capture the different aspects of molecular structure, the Wiener index is the best known one. Vertex version of the Wiener index is the first reported distance-based topological index which was introduced by the Chemist, Harold Wiener, in 1947 [3]. Wiener used his index, for the calculation of the boiling points of alkanes. Using the language which in theoretical Chemistry emerged several decades after Wiener, we may say that Wiener index was conceived as the sum of distances between all pairs of vertices in the molecular graph of an alkane, with the evident aim to provide a measure of the compactness of the respective hydrocarbon molecule. From graph-theoretical point of view, Wiener index of a simple undirected connected graph G is defined as follows:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v|G) \tag{1}$$

where $d(u,v|G)$ denotes the distance between the vertices u and v of G which is defined as the length of any shortest path in G connecting u and v.

Wiener index happens to be one of the most frequently and most successfully employed structural descriptors that can be deduced from the molecular graph. Since 1976, the Wiener number has found a remarkable variety of chemical applications. Physical and chemical properties of organic substances, which can be expected to depend on the area of the molecular surface and/or on the branching of the molecular carbon-atom skeleton, are usually well correlated with Wiener index. Among them are the heats of formation, vaporization and atomization, density, boiling point, critical pressure, refractive index, surface tension and viscosity of various, acyclic and cyclic, saturated and unsaturated as well as aromatic hydrocarbon species, velocity of ultra sound in alkanes and alcohols, rate of electro reduction of chlorobenzenes *etc*. [4]. We refer the reader to [5-7], for more information about the Wiener index.

Edge versions of the Wiener index based on distance between all pairs of edges in a connected graph G were introduced in 2009 [8-10]. In analogy with Eq. (1), the edge-Wiener index of a simple undirected connected graph G needs to be defined as follows:

$$W_e(G) = \sum_{\{e,f\} \subseteq E(G)} d(e,f|G) \tag{2}$$

where $d(e,f|G)$ stands for the distance between the edges e and f of the graph G.

The distance between two edges $e = uv$ and $f = zt$ of the graph G can be defined in two ways [10]. The first distance is denoted by $d_0(e,f|G)$ and defined as follows:

$$d_0(e,f|G)=\begin{cases} d_1(e,f|G)+1 & \text{if } e\neq f \\ 0 & \text{if } e=f \end{cases},$$

where $d_1(e,f|G)=\min\{d(u,z|G),d(u,t|G),d(v,z|G),d(v,t|G)\}$. It is easy to see that $d_0(e,f|G)=d(e,f|L(G))$, where $L(G)$ is the line graph of G.

The second distance is denoted by $d_4(e,f|G)$ and defined as follows:

$$d_4(e,f|G)=\begin{cases} d_2(e,f|G) & \text{if } e\neq f \\ 0 & \text{if } e=f \end{cases},$$

where $d_2(e,f|G)=\max\{d(u,z|G),d(u,t|G),d(v,z|G),d(v,t|G)\}$.

Corresponding to the above distances, two edge versions of the Wiener index can be defined. The first and second edge Wiener indices of G are denoted by $W_{e_0}(G)$ and $W_{e_4}(G)$, respectively and defined as follows [10]:

$$W_{e_i}(G)=\sum_{\{e,f\}\subseteq E(G)} d_i(e,f|G),\quad i\in\{0,4\}.$$

Obviously, $W_{e_0}(G)=W(L(G))$.

In analogy with Eq. (1) and Eq. (2), the vertex-edge Wiener index of G needs to be defined as follows:

$$W_{ve}(G)=\sum_{u\in V(G)}\sum_{e\in E(G)} d(u,e|G) \qquad (3)$$

where $d(u,e|G)$ stands for the distance between the vertex u and the edge e of the graph G.

The distance between the vertex u and the edge $e=ab$ of the graph G can be defined in the two following ways [11]:

$$D_1(u,e|G)=\min\{d(u,a|G),d(u,b|G)\} \text{ and } D_2(u,e|G)=\max\{d(u,a|G),d(u,b|G)\}.$$

Corresponding to the above distances, two vertex-edge versions of the Wiener index can be defined. The first and second vertex-edge Wiener indices of G are denoted by $Min(G)$ and $Max(G)$, respectively and defined as follows [11]:

$$Min(G)=\sum_{u\in V(G)}\sum_{e\in E(G)} D_1(u,e|G)=\sum_{u\in V(G)}\sum_{ab\in E(G)}\min\{d(u,a|G),d(u,b|G)\} \text{ and}$$

$$Max(G)=\sum_{u\in V(G)}\sum_{e\in E(G)} D_2(u,e|G)=\sum_{u\in V(G)}\sum_{ab\in E(G)}\max\{d(u,a|G),d(u,b|G)\}.$$

The indices $Min(G)$ and $Max(G)$ are also called minimum and maximum indices, respectively.

One can easily see that for arbitrary edges $e = uv$ and $f = zt$ of the graph G, the quantities d_i and D_i, $i \in \{1,2\}$, satisfy in the following relations:

$$d_1(e, f|G) = \min\{D_1(u, f|G), D_1(v, f|G)\} = \min\{D_1(z, e|G), D_1(t, e|G)\} \text{ and}$$

$$d_2(e, f|G) = \max\{D_2(u, f|G), D_2(v, f|G)\} = \max\{D_2(z, e|G), D_2(t, e|G)\}.$$

The first relation expresses the relation between the first edge Wiener index $W_{e_0}(G)$ and the first vertex-edge Wiener index $Min(G)$. Similarly, the second relation expresses the relation between the second edge Wiener index $W_{e_4}(G)$ and the second vertex-edge Wiener index $Max(G)$. The vertex-edge Wiener indices play an important role in the computations on the edge Wiener indices. While calculating on the edge Wiener indices $W_{e_0}(G)$ and $W_{e_4}(G)$, their corresponding vertex-edge Wiener indices $Min(G)$ and $Max(G)$ are used frequently. For example, the formulas of the edge Wiener indices of some composite graphs such as the graph of Cartesian product, corona and composition are obtained based on the vertex-edge Wiener indices of the primary graphs [11-14]. Furthermore, when we work on the edge Wiener indices of some classes of chemical graphs and nanostructures, we first need to obtain the vertex-edge Wiener indices of these graphs. For more information, see [15] and [16]. Because of the similarity and relation among the various versions of the Wiener index, it is predicted that the vertex-edge versions of the Wiener index like its vertex and edge versions will find many chemical and mathematical applications in future.

In this paper, we present explicit formulas for computing the first and second vertex-edge Wiener indices of three important classes of molecular graphs containing linear hexagonal chain, cyclic linear hexagonal chain and double linear hexagonal chain.

Discussion and results

In this section, we consider the linear hexagonal chain L_n, cyclic linear hexagonal chain T_n and double linear hexagonal chain B_{2n} and compute the first and second vertex-edge Wiener indices of them.

1. Vertex-edge Wiener indices of linear hexagonal chain

In order to compute the first and second vertex-edge Wiener indices of the linear hexagonal chain L_n, at first we choose a coordinate label for its vertices as shown in Fig. 4.

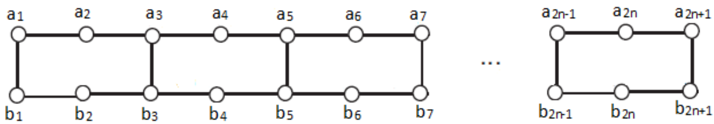

Fig. 4 A coordinate label for vertices of L_n.

Since the vertex-edge Wiener indices are distance-based topological indices, so we need to know the distance between vertices in this graph. So we begin with the following Lemma.

Lemma 1.1 Let $1 \le i, j \le 2n+1$. Then

(i) $d(a_i, a_j | L_n) = d(b_i, b_j | L_n) = |i-j|$.

(ii) $d(a_i, b_j | L_n) = \begin{cases} |i-j|+1 & \text{if } i \ne j \\ 1 & \text{if } i = j \text{ and } i \text{ is odd} \\ 3 & \text{if } i = j \text{ and } i \text{ is even} \end{cases}$.

Proof. (i) Without lost of generality, let $j \ge i$. The shortest path between a_i and a_j is $a_i \to a_{i+1} \to a_{i+2} \to ... \to a_j$ and the shortest path between b_i and b_j is $b_i \to b_{i+1} \to b_{i+2} \to ... \to b_j$. So $d(a_i, a_j | L_n) = d(b_i, b_j | L_n) = j - i$.

(ii) Let $j > i$. A shortest path between a_i and b_j is $a_i \to b_i \to b_{i+1} \to ... \to b_j$, if i is odd and $a_i \to a_{i+1} \to b_{i+1} \to b_{i+2} \to ... \to b_j$, if i is even. So for $j > i$, $d(a_i, b_j | L_n) = j - i + 1$. In the case $i > j$, using a similar method, we conclude that $d(a_i, b_j | L_n) = i - j + 1$. In the case $i = j$, the proof is obvious.□

Definition 1.2 Let $G = (V(G), E(G))$ be a simple undirected connected graph. For $a \in V(G)$, define:

$$D_1(a|G) = \sum_{e \in E(G)} D_1(a, e|G) \text{ and } D_2(a|G) = \sum_{e \in E(G)} D_2(a, e|G).$$

In the following Lemma, we compute the value of $D_2(a_i | L_n)$, for $1 \le i \le 2n+1$.

Lemma 1.3 For $1 \le i \le 2n+1$, we have:

$$D_2(a_i|L_n) = \begin{cases} \frac{5}{2}i^2 - 5(n+1)i + 5n^2 + 11n + \frac{7}{2} & \text{if } i \text{ is odd} \\ \\ \frac{5}{2}i^2 - 5(n+1)i + 5n^2 + 11n + 6 & \text{if } i \text{ is even} \end{cases}.$$

Proof. Let $1 \le i \le 2n+1$. If i is odd, then by the previous Lemma, we have:

$$D_2(a_i|L_n) = \sum_{j=1}^{2n+1} d(a_i, a_j|L_n) + \sum_{\substack{j=1 \\ j \ne i}}^{2n+1} d(a_i, b_j|L_n) + \sum_{j=1}^{n+1} d(a_i, b_{2j-1}|L_n) =$$

$$\sum_{j=1}^{i}(i-j) + \sum_{j=i+1}^{2n+1}(j-i) + \sum_{j=1}^{i-1}(i-j+1) + \sum_{j=i+1}^{2n+1}(j-i+1) + \sum_{j=1}^{\frac{i+1}{2}}(i-2j+2) + \sum_{j=\frac{i+3}{2}}^{n+1}(2j-i),$$

and if i is even, we have:

$$D_2(a_i|L_n) = \sum_{j=1}^{2n+1} d(a_i, a_j|L_n) + \sum_{\substack{j=1 \\ j \ne i-1, i+1}}^{2n+1} d(a_i, b_j|L_n) + d(a_i, b_i|L_n) + \sum_{j=1}^{n+1} d(a_i, b_{2j-1}|L_n) =$$

$$\sum_{j=1}^{i}(i-j) + \sum_{j=i+1}^{2n+1}(j-i) + \sum_{j=1}^{i-2}(i-j+1) + \sum_{j=i+2}^{2n+1}(j-i+1) + 6 + \sum_{j=1}^{\frac{i}{2}}(i-2j+2) + \sum_{j=\frac{i+2}{2}}^{n+1}(2j-i).$$

After computing each summation, we can obtain the desire result.□

Lemma 1.4 For $1 \le i \le 2n+1$, $D_2(a_i|L_n) - D_1(a_i|L_n) = 5n+1$.

Proof. Let $1 \le i \le 2n+1$. If i is odd, then

$$D_1(a_i|L_n) = \sum_{j=2}^{2n} d(a_i, a_j|L_n) + \sum_{j=2}^{2n} d(a_i, b_j|L_n) + d(a_i, b_i|L_n) + \sum_{j=1}^{n+1} d(a_i, a_{2j-1}|L_n),$$

and if i is even, then

$$D_1(a_i|L_n) = \sum_{j=2}^{2n} d(a_i, a_j|L_n) + \sum_{\substack{j=2 \\ j \ne i}}^{2n} d(a_i, b_j|L_n) + d(a_i, b_{i-1}|L_n) + d(a_i, b_{i+1}|L_n) + \sum_{j=1}^{n+1} d(a_i, a_{2j-1}|L_n).$$

Now according to the proof of the previous lemma, the proof is clear.□

Now, we are ready to obtain the vertex-edge Wiener indices of the linear hexagonal chain L_n in the following Theorem.

Theorem 1.5

(i) $Max(L_n)=\frac{1}{3}(40n^3+102n^2+68n+6)$.

(ii) $Min(L_n)=\frac{1}{3}(40n^3+42n^2+26n)$.

Proof. **(i)** The symmetry of the graph L_n implies that for every $1\le i\le 2n+1$, $D_2(a_i|L_n)=D_2(b_i|L_n)$. So

$$Max(L_n)=2\sum_{i=1}^{2n+1}D_2(a_i|L_n)=2[\sum_{i=1}^{n+1}D_2(a_{2i-1}|L_n)+\sum_{i=1}^{n}D_2(a_{2i}|L_n)].$$

Now, using Lemma 1.3, the proof is straightforward.

(ii) Using Lemma 1.4, we have:

$$Min(L_n)=2\sum_{i=1}^{2n+1}D_1(a_i|L_n)=2\sum_{i=1}^{2n+1}[D_2(a_i|L_n)-(5n+1)]=Max(L_n)-2(5n+1)(2n+1).$$

Now by part (i) of the Theorem, the proof is obvious.□

2. Vertex-edge Wiener indices of cyclic linear hexagonal chain

In order to find the first and second vertex-edge Wiener indices of the cyclic linear hexagonal chain T_n, at first consider a coordinate label for its vertices as shown in Fig. 5.

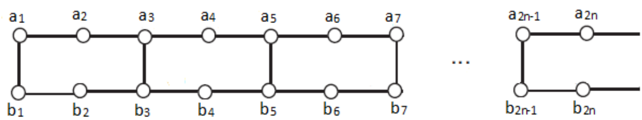

Fig. 5 Two dimensional lattice of T_n with a coordinate label for its vertices.

In the following Lemma, we obtain the distance between all vertices of T_n with the vertices a_1 and a_2.

Lemma 2.1 Let $1\le i\le 2n$. Then

(i) $$d(a_1,a_i|T_n)=\begin{cases} i-1 & if\ 1\le i\le n+1 \\ 2n+1-i & if\ n+2\le i\le 2n \end{cases}.$$

(ii) $$d(a_1,b_i|T_n)=\begin{cases} i & if\ 1\le i\le n+1 \\ 2n+2-i & if\ n+2\le i\le 2n \end{cases}.$$

(iii) $$d(a_2,a_i|T_n)=\begin{cases}1 & \text{if } i=1\\ i-2 & \text{if } 2\le i\le n+2\\ 2n+2-i & \text{if } n+3\le i\le 2n\end{cases}.$$

(iv) $$d(a_2,b_i|T_n)=\begin{cases}2 & \text{if } i=1\\ 3 & \text{if } i=2\\ i-1 & \text{if } 3\le i\le n+2\\ 2n+3-i & \text{if } n+3\le i\le 2n\end{cases}.$$

Proof. (i) The shortest path between a_1 and a_i is

$a_1\to a_2\to\ldots\to a_i$, if $1\le i\le n+1$ and $a_i\to a_{i+1}\to\ldots\to a_{2n}\to a_1$, if $n+2\le i\le 2n$. So

$$d(a_1,a_i|T_n)=\begin{cases}i-1 & \text{if } 1\le i\le n+1\\ 2n+1-i & \text{if } n+2\le i\le 2n\end{cases}.$$

(ii) A shortest path between a_1 and b_i is $a_1\to b_1\to b_2\to\ldots\to b_i$, if $1\le i\le n+1$ and $b_i\to b_{i+1}\to\ldots\to b_{2n}\to b_1\to a_1$, if $n+2\le i\le 2n$. So

$$d(a_1,b_i|T_n)=\begin{cases}i & \text{if } 1\le i\le n+1\\ 2(n+1)-i & \text{if } n+2\le i\le 2n\end{cases}.$$

(iii) It is clear that $d(a_2,a_1|T_n)=1$. The shortest path between a_2 and a_i is

$a_2\to a_3\to\ldots\to a_i$, if $2\le i\le n+2$ and $a_i\to a_{i+1}\to\ldots\to a_{2n}\to a_1\to a_2$, if $n+3\le i\le 2n$.

So

$$d(a_2,a_i|T_n)=\begin{cases}1 & \text{if } i=1\\ i-2 & \text{if } 2\le i\le n+2\\ 2(n+1)-i & \text{if } n+3\le i\le 2n\end{cases}.$$

(iv) It is clear that $d(a_2,b_1|T_n)=2$ and $d(a_2,b_2|T_n)=3$. A shortest path between a_2 and b_i is $a_2\to a_3\to b_3\to b_4\to\ldots\to b_i$, if $3\le i\le n+2$ and $b_i\to b_{i+1}\to\ldots\to b_{2n}\to b_1\to a_1\to a_2$, if $n+3\le i\le 2n$. So

$$d(a_2,b_i|T_n)=\begin{cases}2 & \text{if } i=1\\ 3 & \text{if } i=2\\ i-1 & \text{if } 3\le i\le n+2\\ 2n+3-i & \text{if } n+3\le i\le 2n\end{cases}.\square$$

Lemma 2.2 Let $i\in\{1,2\}$. If n is odd, then

$$D_1(a_i|T_n)=\begin{cases}\frac{5}{2}n^2-\frac{1}{2} & if\ \ i=1\\ \frac{5}{2}n^2+\frac{5}{2} & if\ \ i=2\end{cases} \text{ and } D_2(a_i|T_n)=\begin{cases}\frac{5}{2}n^2+5n-\frac{1}{2} & if\ \ i=1\\ \frac{5}{2}n^2+5n+\frac{5}{2} & if\ \ i=2\end{cases}.$$

If n is even, then

$$D_1(a_i|T_n)=\begin{cases}\frac{5}{2}n^2 & if\ \ i=1\\ \frac{5}{2}n^2+2 & if\ \ i=2\end{cases} \text{ and } D_2(a_i|T_n)=\begin{cases}\frac{5}{2}n^2+5n & if\ \ i=1\\ \frac{5}{2}n^2+5n+2 & if\ \ i=2\end{cases}.$$

Proof. It is easy to see that:

$$D_1(a_1|T_n)=\sum_{\substack{i=1\\ i\neq n+1}}^{2n}d(a_1,a_i|T_n)+d(a_1,b_1|T_n)+\sum_{\substack{i=1\\ i\neq n+1}}^{2n}d(a_1,b_i|T_n)+\sum_{i=1}^{n}d(a_1,a_{2i-1}|T_n),$$

$$D_1(a_2|T_n)=\sum_{\substack{i=1\\ i\neq n+2}}^{2n}d(a_2,a_i|T_n)+2d(a_2,b_1|T_n)+2d(a_2,b_3|T_n)+\sum_{\substack{i=4\\ i\neq n+2}}^{2n}d(a_2,b_i|T_n)+\sum_{i=1}^{n}d(a_2,a_{2i-1}|T_n),$$

$$D_2(a_1|T_n)=\sum_{i=1}^{2n}d(a_1,a_i|T_n)+d(a_1,a_{n+1}|T_n)+\sum_{i=2}^{2n}d(a_1,b_i|T_n)+d(a_1,b_{n+1}|T_n)+\sum_{i=1}^{n}d(a_1,b_{2i-1}|T_n) \text{ and}$$

$$D_2(a_2|T_n)=\sum_{i=1}^{2n}d(a_2,a_i|T_n)+d(a_2,a_{n+2}|T_n)+2d(a_2,b_2|T_n)+\sum_{i=4}^{2n}d(a_2,b_i|T_n)+d(a_2,b_{n+2}|T_n)+$$
$$\sum_{i=1}^{n}d(a_2,b_{2i-1}|T_n).$$

Now, using the previous lemma, we have:

$$D_1(a_1|T_n)=\sum_{i=1}^{n}(i-1)+\sum_{i=n+2}^{2n}(2n+1-i)+1+\sum_{i=1}^{n}i+\sum_{i=n+2}^{2n}(2n+2-i)+$$
$$\begin{cases}\sum_{i=1}^{\frac{n+1}{2}}(2i-2)+\sum_{i=\frac{n+3}{2}}^{n}(2n+2-2i) & if\ n\ is\ odd\\ \sum_{i=1}^{\frac{n+2}{2}}(2i-2)+\sum_{i=\frac{n+4}{2}}^{n}(2n+2-2i) & if\ n\ is\ even\end{cases},$$

$$D_1(a_2|T_n)=1+\sum_{i=2}^{n+1}(i-2)+\sum_{i=n+3}^{2n}(2n+2-i)+4+4+\sum_{i=4}^{n+1}(i-1)+\sum_{i=n+3}^{2n}(2n+3-i)+$$
$$\begin{cases}1+\sum_{i=2}^{\frac{n+3}{2}}(2i-3)+\sum_{i=\frac{n+5}{2}}^{n}(2n+3-2i) & if\ n\ is\ odd\\ 1+\sum_{i=2}^{\frac{n+2}{2}}(2i-3)+\sum_{i=\frac{n+4}{2}}^{n}(2n+3-2i) & if\ n\ is\ even\end{cases},$$

$$D_2(a_1|T_n)=\sum_{i=1}^{n+1}(i-1)+n+\sum_{i=n+2}^{2n}(2n+1-i)+\sum_{i=2}^{n+1}i+(n+1)+\sum_{i=n+2}^{2n}(2n+2-i)+$$
$$\begin{cases}\sum_{i=1}^{\frac{n+1}{2}}(2i-1)+\sum_{i=\frac{n+3}{2}}^{n}(2n+3-2i) & \text{if } n \text{ is odd}\\ \sum_{i=1}^{\frac{n+2}{2}}(2i-1)+\sum_{i=\frac{n+4}{2}}^{n}(2n+3-2i) & \text{if } n \text{ is even}\end{cases},$$

and

$$D_2(a_2|T_n)=1+\sum_{i=2}^{n+2}(i-2)+n+\sum_{i=n+3}^{2n}(2n+2-i)+6+\sum_{i=4}^{n+2}(i-1)+(n+1)+\sum_{i=n+3}^{2n}(2n+3-i)+$$
$$\begin{cases}2+\sum_{i=2}^{\frac{n+3}{2}}(2i-2)+\sum_{i=\frac{n+5}{2}}^{n}(2n+4-2i) & \text{if } n \text{ is odd}\\ 2+\sum_{i=2}^{\frac{n+2}{2}}(2i-2)+\sum_{i=\frac{n+4}{2}}^{n}(2n+4-2i) & \text{if } n \text{ is even}\end{cases}.$$

Now, the proof is straightforward.□

Below, we compute the first and second vertex-edge Wiener indices of the graph T_n.

Theorem 2.3

$$Min(T_n)=2n(5n^2+2) \text{ and } Max(T_n)=2n(5n^2+10n+2).$$

Proof. Using the previous Lemma, we have:

$Min(T_n)=2n(D_1(a_1|T_n)+D_1(a_2|T_n))=2n(5n^2+2)$ and

$Max(T_n)=2n(D_2(a_1|T_n)+D_2(a_2|T_n))=2n(5n^2+10n+2)$. □

3. Vertex-edge Wiener indices of double linear hexagonal chain

In order to compute the first and second vertex-edge Wiener indices of the double linear hexagonal chain B_{2n}, at first we choose a coordinate label for its vertices as shown in Fig. 6.

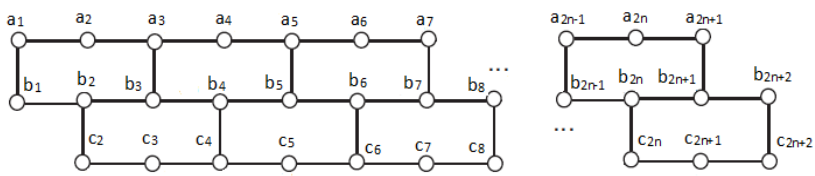

Fig. 6 A coordinate label for vertices of B_{2n}.

We begin with the following Lemma.

Lemma 3.1

(i) For $1 \le i, j \le 2n+1$, $d(a_i, a_j | B_{2n}) = |i-j|$.

(ii) For $1 \le i, j \le 2n+2$, $d(b_i, b_j | B_{2n}) = |i-j|$.

(iii) For $2 \le i, j \le 2n+2$, $d(c_i, c_j | B_{2n}) = |i-j|$.

(iv) For $1 \le i \le 2n+1$ and $1 \le j \le 2n+2$,

$$d(a_i, b_j | B_{2n}) = \begin{cases} |i-j|+1 & \text{if } i \ne j \\ 1 & \text{if } i = j \text{ and } i \text{ is odd} \\ 3 & \text{if } i = j \text{ and } i \text{ is even} \end{cases}.$$

(v) For $1 \le i \le 2n+2$ and $2 \le j \le 2n+2$,

$$d(b_i, c_j | B_{2n}) = \begin{cases} |i-j|+1 & \text{if } i \ne j \\ 3 & \text{if } i = j \text{ and } i \text{ is odd} \\ 1 & \text{if } i = j \text{ and } i \text{ is even} \end{cases}.$$

(vi) For $1 \le i \le 2n+1$ and $2 \le j \le 2n+2$,

$$d(a_i, c_j | B_{2n}) = \begin{cases} |i-j|+2 & \text{if } i \ne j \text{ and } i \text{ is odd} \\ |i-j|+2 & \text{if } j \notin \{i-1, i, i+1\} \text{ and } i \text{ is even} \\ 4 & \text{if } i = j \\ 5 & \text{if } j \in \{i-1, i+1\} \text{ and } i \text{ is even} \end{cases}.$$

Proof. Proof is similar to the proof of Lemma1.1.□

In the following Lemma, we compute the value of $D_2(a_i | B_{2n})$ and $D_2(b_j | B_{2n})$, for $1 \le i \le 2n+1$ and $1 \le j \le 2n+2$.

Lemma 3.2

(i) For $1 \le i \le 2n+1$, we have:

$$D_2(a_i | B_{2n}) = \begin{cases} 8n^2 + 19n + 6 & \text{if } i = 1 \\ 4i^2 - (8n+12)i + 8n^2 + 27n + 17 & \text{if } i \ne 1 \text{ and } i \text{ is odd} \\ 8n^2 + 11n + 14 & \text{if } i = 2 \\ 4i^2 - (8n+12)i + 8n^2 + 27n + 25 & \text{if } i \ne 2 \text{ and } i \text{ is even} \end{cases}.$$

(ii) For $1 \le i \le 2n+2$, we have:

$$D_2(b_i|B_{2n})=\begin{cases}8n^2+16n+7 & if\ \ i\in\{1,2n+2\}\\ 4i^2-(8n+12)i+8n^2+24n+15 & otherwise\end{cases}.$$

Proof. By previous Lemma, we have:

(i) $D_2(a_1|B_{2n})=\sum_{j=2}^{2n+1}d(a_1,a_j|B_{2n})+\sum_{j=2}^{2n+2}d(a_1,b_j|B_{2n})+\sum_{j=3}^{2n+2}d(a_1,c_j|B_{2n})+$

$$\sum_{j=1}^{n+1}d(a_1,b_{2j-1}|B_{2n})+\sum_{j=1}^{n+1}d(a_1,c_{2j}|B_{2n})=\sum_{j=2}^{2n+1}(j-1)+\sum_{j=2}^{2n+2}j+\sum_{j=3}^{2n+2}(j+1)+\sum_{j=1}^{n+1}(2j-1)+\sum_{j=1}^{n+1}(2j+1),$$

and

$$D_2(a_2|B_{2n})=d(a_2,a_1|B_{2n})+\sum_{j=3}^{2n+1}d(a_2,a_j|B_{2n})+2d(a_2,b_2|B_{2n})+\sum_{j=4}^{2n+2}d(a_2,b_j|B_{2n})+$$

$$2d(a_2,c_3|B_{2n})+\sum_{j=5}^{2n+2}d(a_2,c_j|B_{2n})+\sum_{j=1}^{n+1}d(a_1,b_{2j-1}|B_{2n})+\sum_{j=1}^{n+1}d(a_1,c_{2j}|B_{2n})=$$

$$1+\sum_{j=3}^{2n+1}(j-2)+2\times3+\sum_{j=4}^{2n+2}(j-1)+2\times5+\sum_{j=5}^{2n+2}j+2+\sum_{j=2}^{n+1}(2j-2)+4+\sum_{j=2}^{n+1}2j.$$

If $i\neq1$ and i is odd, then the calculation of $D_2(a_i|B_{2n})$ is as follows:

$$D_2(a_i|B_{2n})=\sum_{j=1}^{i-1}d(a_i,a_j|B_{2n})+\sum_{j=i+1}^{2n+1}d(a_i,a_j|B_{2n})+\sum_{j=1}^{i-1}d(a_i,b_j|B_{2n})+$$

$$\sum_{j=i+1}^{2n+2}d(a_i,b_j|B_{2n})+\sum_{j=2}^{i-2}d(a_i,c_j|B_{2n})+2d(a_i,c_i|B_{2n})+\sum_{j=i+2}^{2n+2}d(a_i,c_j|B_{2n})+$$

$$\sum_{j=1}^{n+1}d(a_i,b_{2j-1}|B_{2n})+\sum_{j=1}^{n+1}d(a_i,c_{2j}|B_{2n})=\sum_{j=1}^{i-1}(i-j)+\sum_{j=i+1}^{2n+1}(j-i)+\sum_{j=1}^{i-1}(i-j+1)+$$

$$\sum_{j=i+1}^{2n+2}(j-i+1)+\sum_{j=2}^{i-2}(i-j+2)+2\times4+\sum_{j=i+2}^{2n+2}(j-i+2)+\sum_{j=1}^{\frac{i+1}{2}}(i-2j+2)+\sum_{j=\frac{i+3}{2}}^{n+1}(2j-i)+$$

$$\sum_{j=1}^{\frac{i-1}{2}}(i-2j+2)+\sum_{j=\frac{i+1}{2}}^{n+1}(2j-i+2),$$

if $i\neq2$ and i is even, then the calculation of $D_2(a_i|B_{2n})$ is as follows:

$$D_2(a_i|B_{2n})=\sum_{j=1}^{i-1}d(a_i,a_j|B_{2n})+\sum_{j=i+1}^{2n+1}d(a_i,a_j|B_{2n})+\sum_{j=1}^{i-2}d(a_i,b_j|B_{2n})+2d(a_i,b_i|B_{2n})+$$

$$\sum_{j=i+2}^{2n+2}d(a_i,b_j|B_{2n})+\sum_{j=2}^{i-3}d(a_i,c_j|B_{2n})+2d(a_i,c_{i-1}|B_{2n})+2d(a_i,c_{i+1}|B_{2n})+\sum_{j=i+3}^{2n+2}d(a_i,c_j|B_{2n})+$$

$$\sum_{j=1}^{n+1} d(a_i, b_{2j-1}|B_{2n}) + \sum_{j=1}^{n+1} d(a_i, c_{2j}|B_{2n}) = \sum_{j=1}^{i-1}(i-j) + \sum_{j=i+1}^{2n+1}(j-i) + \sum_{j=1}^{i-2}(i-j+1) + 2\times 3 +$$

$$\sum_{j=i+2}^{2n+2}(j-i+1) + \sum_{j=2}^{i-3}(i-j+2) + 2\times 5 + 2\times 5 + \sum_{j=i+3}^{2n+2}(j-i+2) + \sum_{j=1}^{\frac{i}{2}}(i-2j+2) + \sum_{j=\frac{i+2}{2}}^{n+1}(2j-i) +$$

$$\sum_{j=1}^{\frac{i-2}{2}}(i-2j+2) + 4 + \sum_{j=\frac{i+2}{2}}^{n+1}(2j-i+2).$$

Now, the proof is straightforward.

(ii) Similar to the proof of the previous part, we have:

$$D_2(b_1|B_{2n}) = \sum_{j=2}^{2n+1} d(b_1, a_j|B_{2n}) + \sum_{j=2}^{2n+2} d(b_1, b_j|B_{2n}) + \sum_{j=3}^{2n+2} d(b_1, c_j|B_{2n}) +$$

$$\sum_{j=1}^{n+1} d(b_1, a_{2j-1}|B_{2n}) + \sum_{j=1}^{n+1} d(b_1, c_{2j}|B_{2n}) = \sum_{j=2}^{2n+1} j + \sum_{j=2}^{2n+2}(j-1) + \sum_{j=3}^{2n+2} j + \sum_{j=1}^{n+1}(2j-1) + \sum_{j=1}^{n+1} 2j.$$

By the symmetry of B_{2n}, we have $D_2(b_1|B_{2n}) = D_2(b_{2n+2}|B_{2n})$.

If $i \neq 1$ and i is odd, then the calculation of $D_2(b_i|B_{2n})$ is as follows:

$$D_2(b_i|B_{2n}) = \sum_{j=1}^{i-1} d(b_i, a_j|B_{2n}) + \sum_{j=i+1}^{2n+1} d(b_i, a_j|B_{2n}) + \sum_{j=1}^{i-1} d(b_i, b_j|B_{2n}) +$$

$$\sum_{j=i+1}^{2n+2} d(b_i, b_j|B_{2n}) + \sum_{j=2}^{i-2} d(b_i, c_j|B_{2n}) + 2d(b_i, c_i|B_{2n}) + \sum_{j=i+2}^{2n+2} d(b_i, c_j|B_{2n}) +$$

$$\sum_{j=1}^{n+1} d(b_i, a_{2j-1}|B_{2n}) + \sum_{j=1}^{n+1} d(b_i, c_{2j}|B_{2n}) = \sum_{j=1}^{i-1}(i-j+1) + \sum_{j=i+1}^{2n+1}(j-i+1) + \sum_{j=1}^{i-1}(i-j) +$$

$$\sum_{j=i+1}^{2n+2}(j-i) + \sum_{j=2}^{i-2}(i-j+1) + 2\times 3 + \sum_{j=i+2}^{2n+2}(j-i+1) + \sum_{j=1}^{\frac{i+1}{2}}(i-2j+2) + \sum_{j=\frac{i+3}{2}}^{n+1}(2j-i) +$$

$$\sum_{j=1}^{\frac{i-1}{2}}(i-2j+1) + \sum_{j=\frac{i+1}{2}}^{n+1}(2j-i+1),$$

if $i \neq 2n+2$ and i is even, then the calculation of $D_2(b_i|B_{2n})$ is as follows:

$$D_2(b_i|B_{2n}) = \sum_{j=1}^{i-2} d(b_i, a_j|B_{2n}) + 2d(b_i, a_i|B_{2n}) + \sum_{j=i+2}^{2n+1} d(b_i, a_j|B_{2n}) + \sum_{j=1}^{i-1} d(b_i, b_j|B_{2n}) +$$

$$\sum_{j=i+1}^{2n+2} d(b_i, b_j|B_{2n}) + \sum_{j=2}^{i-1} d(b_i, c_j|B_{2n}) + \sum_{j=i+1}^{2n+2} d(b_i, c_j|B_{2n}) + \sum_{j=1}^{n+1} d(b_i, a_{2j-1}|B_{2n}) + \sum_{j=1}^{n+1} d(b_i, c_{2j}|B_{2n}) =$$

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

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

According to the above computation, we can obtain the desire results. □

Lemma 3.3

(i) For $1\le i\le 2n+1$, $D_2(a_i|B_{2n})-D_1(a_i|B_{2n})=8n+3$.

(ii) For $1\le i\le 2n+2$, $D_2(b_i|B_{2n})-D_1(b_i|B_{2n})=8n+3$.

Proof. By the previous Lemma, it is enough to compute the values of $D_1(a_i|B_{2n})$ and $D_1(b_j|B_{2n})$, for $1\le i\le 2n+1$ and $1\le j\le 2n+2$.

(i) We compute:

$$D_1(a_1|B_{2n})=\sum_{j=2}^{2n}d(a_1,a_j|B_{2n})+\sum_{j=1}^{2n+1}d(a_1,b_j|B_{2n})+\sum_{j=2}^{2n+1}d(a_1,c_j|B_{2n})+\sum_{j=1}^{n+1}d(a_1,a_{2j-1}|B_{2n})+$$

$$\sum_{j=1}^{n+1}d(a_1,b_{2j}|B_{2n}),\text{ and}$$

$$D_1(a_2|B_{2n})=\sum_{j=3}^{2n}d(a_2,a_j|B_{2n})+d(a_2,b_1|B_{2n})+d(a_2,b_3|B_{2n})+\sum_{j=3}^{2n+1}d(a_2,b_j|B_{2n})+d(a_2,c_2|B_{2n})+$$

$$d(a_2,c_4|B_{2n})+\sum_{j=4}^{2n+1}d(a_2,c_j|B_{2n})+\sum_{j=1}^{n+1}d(a_2,a_{2j-1}|B_{2n})+\sum_{j=1}^{n+1}d(a_2,b_{2j}|B_{2n}),$$

If $i\ne 1$ and i is odd, then the calculation of $D_1(a_i|B_{2n})$ is as follows:

$$D_1(a_i|B_{2n})=\sum_{j=2}^{i-1}d(a_i,a_j|B_{2n})+\sum_{j=i+1}^{2n}d(a_i,a_j|B_{2n})+\sum_{j=2}^{i-1}d(a_i,b_j|B_{2n})+2d(a_i,b_i|B_{2n})+$$

$$\sum_{j=i+1}^{2n+1}d(a_i,b_j|B_{2n})+\sum_{j=3}^{i-1}d(a_i,c_j|B_{2n})+d(a_i,c_{i-1}|B_{2n})+d(a_i,c_{i+1}|B_{2n})+\sum_{j=i+1}^{2n+1}d(a_i,c_j|B_{2n})+$$

$$\sum_{j=1}^{n+1}d(a_i,a_{2j-1}|B_{2n})+\sum_{j=1}^{n+1}d(a_i,b_{2j}|B_{2n}),$$

if $i\ne 2$ and i is even, then the calculation of $D_1(a_i|B_{2n})$ is as follows:

$$D_1(a_i|B_{2n}) = \sum_{j=2}^{i-1} d(a_i,a_j|B_{2n}) + \sum_{j=i+1}^{2n} d(a_i,a_j|B_{2n}) + \sum_{j=2}^{i-1} d(a_i,b_j|B_{2n}) +$$
$$d(a_i,b_{i-1}|B_{2n}) + d(a_i,b_{i+1}|B_{2n}) + \sum_{j=i+1}^{2n+1} d(a_i,b_j|B_{2n}) + \sum_{j=3}^{i-2} d(a_i,c_j|B_{2n}) + d(a_i,c_{i-2}|B_{2n}) +$$
$$2d(a_i,c_i|B_{2n}) + d(a_i,c_{i+2}|B_{2n}) + \sum_{j=i+2}^{2n+1} d(a_i,c_j|B_{2n}) + \sum_{j=1}^{n+1} d(a_i,a_{2j-1}|B_{2n}) + \sum_{j=1}^{n+1} d(a_i,b_{2j}|B_{2n}).$$

Now according to the proof of part (i) of the previous lemma, part (i) holds.

(ii) Similar to the proof of part (i), we have:

$$D_1(b_1|B_{2n}) = \sum_{j=1}^{2n} d(b_1,a_j|B_{2n}) + \sum_{j=1}^{2n+1} d(b_1,b_j|B_{2n}) + \sum_{j=2}^{2n+1} d(b_1,c_j|B_{2n}) + \sum_{j=1}^{n+1} d(b_1,b_{2j-1}|B_{2n}) +$$
$$\sum_{j=1}^{n+1} d(b_1,b_{2j}|B_{2n}).$$

By the symmetry of B_{2n}, $D_1(b_1|B_{2n}) = D_1(b_{2n+2}|B_{2n})$.

If $i \neq 1$ and i is odd, then the calculation of $D_1(b_i|B_{2n})$ is as follows:

$$D_1(b_i|B_{2n}) = \sum_{j=2}^{i-1} d(b_i,a_j|B_{2n}) + 2d(b_i,a_i|B_{2n}) + \sum_{j=i+1}^{2n} d(b_i,a_j|B_{2n}) + \sum_{j=2}^{i-1} d(b_i,b_j|B_{2n}) +$$
$$\sum_{j=i+1}^{2n+1} d(b_i,b_j|B_{2n}) + \sum_{j=3}^{i-1} d(b_i,c_j|B_{2n}) + d(b_i,c_{i-1}|B_{2n}) + d(b_i,c_{i+1}|B_{2n}) + \sum_{j=i+1}^{2n+1} d(b_i,c_j|B_{2n}) +$$
$$\sum_{j=1}^{n+1} d(b_i,b_{2j-1}|B_{2n}) + \sum_{j=1}^{n+1} d(b_i,b_{2j}|B_{2n}),$$

if $i \neq 2n+2$ and i is even, then the calculation of $D_1(b_i|B_{2n})$ is as follows:

$$D_1(b_i|B_{2n}) = \sum_{j=2}^{i-1} d(b_i,a_j|B_{2n}) + d(b_i,a_{i-1}|B_{2n}) + d(b_i,a_{i+1}|B_{2n}) + \sum_{j=i+1}^{2n} d(b_i,a_j|B_{2n}) + \sum_{j=2}^{i-1} d(b_i,b_j|B_{2n}) +$$
$$\sum_{j=i+1}^{2n+1} d(b_i,b_j|B_{2n}) + \sum_{j=3}^{i-1} d(b_i,c_j|B_{2n}) + 2d(b_i,c_i|B_{2n}) + \sum_{j=i+1}^{2n+1} d(b_i,c_j|B_{2n}) + \sum_{j=1}^{n+1} d(b_i,b_{2j-1}|B_{2n}) +$$
$$\sum_{j=1}^{n+1} d(b_i,b_{2j}|B_{2n}).$$

Now according to the proof of part (ii) of the previous lemma, part (ii) holds. □

Now, we use Lemmas 3.2 and 3.3 to obtain the first and second vertex-edge Wiener indices of B_{2n} in the following Theorem.

Theorem 3.4

(i) $Max(B_{2n}) = 32n^3 + 116n^2 + 128n + 14$.

(ii) $Min(B_{2n}) = 32n^3 + 68n^2 + 78n + 2$.

Proof. (i) The symmetry of the graph B_{2n} implies that, for every $1 \le i \le 2n+1$, $D_2(a_i|B_{2n}) = D_2(c_{2n+3-i}|B_{2n})$. Hence

$$Max(B_{2n}) = 2[\sum_{i=1}^{2n+1} D_2(a_i|B_{2n}) + \sum_{i=1}^{n+1} D_2(b_i|B_{2n})] = 2[\sum_{i=1}^{n+1} D_2(a_{2i-1}|B_{2n}) + \sum_{i=1}^{n} D_2(a_{2i}|B_{2n}) +$$
$$D_2(b_1|B_{2n}) + \sum_{i=2}^{n+1} D_2(b_i|B_{2n})].$$

Now, using Lemma 3.2, the proof is straightforward.

(ii) Using Lemma 3.3, we have:

$$Min(B_{2n}) = 2[\sum_{i=1}^{2n+1} D_1(a_i|B_{2n}) + \sum_{i=1}^{n+1} D_1(b_i|B_{2n})] =$$
$$2\{\sum_{i=1}^{2n+1}[D_2(a_i|B_{2n}) - (8n+3)] + \sum_{i=1}^{n+1}[D_2(b_i|B_{2n}) - (8n+3)]\} = Max(B_{2n}) - 2(8n+3)(3n+2).$$

Now by part (i), the proof is obvious.□

Conclusion

In this paper, we computed the vertex-edge Wiener indices of some classes of molecular graphs made by hexagons. Nevertheless, there are still many classes of chemically interesting and relevant graphs not covered by our approach. So, it would be interesting to find explicit formulas for the vertex-edge Wiener indices of various classes of chemical graphs and nanostructures.

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