The hyper-Wiener index of one-pentagonal carbon nanocone

M.H.Khalifeh, M.R.Darafsheh*,Hassan Jolany

School of Mathematics, College of Science, University of Tehran, Tehran .Iran.

E-mail addresses: khalife@khayam.ut.ac.ir(M.H.Khalifeh), darafsheh@ut.ac.ir(M.R.Darafsheh), Hassan.jolany@khayam.ut.ac.ir (Hassan Jolany)

Abstract:

one-pentagonal carbon nanocone consists of one pentagone as its core surrounded by layers of hexagons .if there are $n$ layers ,then the graph of this molecules is denoted by $G_n$. In This paper our aim is to calculate the hyper-Wiener index of $G_n$ explicitly .

1. Introduction and Preliminary results

Let $G$ be a simple connected graph. The vertex set and edge set of $G$ are denoted by $V(G)$ and $E(G)$ respectively. The distance between two vertices $u$ and $v$ in $V(G)$ is denoted by $d_G(u,v)$ and is equal to the length of the shortest path from $u$ to $v$.

The Wiener index of $G$ is denoted by $W(G)$ and is defined by $W(G) = \sum_{(u,v)\in E(G)} d_G(u,v)$. The name Wiener index is usual for chemical graphs, that is the graph of a chemical molecule, because Harold Wiener was the first person who considered this invariant for a Chemical graph [1]. Wiener used this index only for acyclic molecules in a slightly different way. But the definition of the Wiener index in terms of distances between vertices of a graph for the first time was given by Hosoya in [2]. The Wiener index of graphs is extensively studied in [3], [4] and [5]. In [6] new method are invented to calculate the Wiener index of a graph. a generalization of the concept of the Wiener index in recent chemical studies is the hyper-Wiener index.

*Corresponding author (e-mail: daraf@khayam.ut.ac.ir)

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Which was put forward in [7] and since then many research papers are written about this index. For example we can refer the reader to [8], [9] and [10]. We will define the hyper-wiener index of a graph $G$ as follow

**Definition 1.** Let $G$ be a simple connected graph with vertex set $V(G)$. For a real number $\lambda$ define

$$W_{\lambda}(G) = \sum_{u,v \in V(G)} d_G(u,v)^{\lambda}$$

Then $W_{1}(G)$ is the Wiener index of $G$, and the hyper-Wiener index of $G$ which is denoted by $WW(G)$ is defined by

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} \left( (d_G(u,v)^2 + d_G(u,v)) \right) = \frac{1}{2} \left( W_2(G) + W_1(G) \right)$$

Some more concepts are needed for our further work which are defined below.

**Definition 2.** Let $G$ be a simple connected graph with vertex set $V(G)$. For $F \subseteq V(G)$ the following quantity is defined:

$$D_G^{\lambda}(F) = \sum_{u \in F} \sum_{v \in V(G) \setminus F} d_G(u,v)^{\lambda}$$

Where $\lambda$ is a real number. If $K = V(G)$, then we set $D^\lambda_G(F,V(G)) = D^\lambda(F,G)$

**Definition 3.** Let $G$ be a simple connected graph. The subgraph $H$ of $G$ is called isometric and is written $H \ll G$ if $d_G(u,v) = d_H(u,v)$ for all $u, v \in V(H)$.

**Definition 4.** Let $G$ be a simple connected graph, the subgraph $H$ of $G$ is called convex if it contains all the shortest paths in $G$ between each pair of its vertices.

Referring to the above concepts if $H \ll G$, then it is evident that $D^\lambda_H(V(H),V(H)) = 2W^\lambda_H(H)$ and if $\{V_k\}_{k=1}^n$ is a partition of $V(G)$, then

$$W^\lambda_A(G) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n D^\lambda_G(V_i,V_j)$$

To state the next result we need some explanation. Let $G$ be a simple connected graph. If $e \in E(G)$, then $G - e$ stands for the graph remaining from $G$ by deleting $e$ not its ends. Similarly, if $F \subseteq E(G)$, then $G - F$ is defined to be the graph remaining from $G$ by deleting all the edges in $F$ not the end vertices.

**Theorem 1.** Let $G$ be a simple connected graph, if $\{F_i\}_{i=1}^n$ is a partition of $E(G)$ such that each of $(G - F_i)$ is a graph with two convex connected components $G^1_i$ and $G^2_i$, then
\[
W_{\lambda+1}(G) = nW_\lambda(G) - \sum_{i=1}^{n} \left( W_\lambda(G^i_1) + W_\lambda(G^i_2) \right)
\]

Where \( \lambda \) is a real number.

**Proof.** See [11].

**Theorem 1.** Let \( G \) be a simple connected graph, if \( \{F_i\}_{i=1}^{n} \) is a partition of \( E(G) \) such that each of \( (G - F_i) \) is a graph with two convex connected components \( G^i_1 \) and \( G^i_2 \), then the Wiener index of \( G \) is:

\[
W(G) = \sum_{i=1}^{n} |V(G^i_1)||V(G^i_2)|
\]

**Proof.** See [11]

### 2. Computing with subgraphs

As we mentioned earlier our aim is to calculate the hyper-Wiener index of the one-pentagonal carbon nanocone. The graph of this molecule consist one pentagone surrounded by layers of hexagons. If there are \( n \) layers, then this graph is denoted by \( G_n \).

In the following the graph of \( G_6 \) is drawn:

Figur1: The graph of \( G_6 \)

Our calculations are based on Theorems 1 and 2. For the starting point we calculate the Wiener index of the auxiliary graphs which are denoted by \( Z_{n,k}, M_{n,k}, Z_{n,k,l} \) and \( A_n \).

First we explain the above graph and draw them in special cases of \( n, k \) and \( l \).

**\( Z_{n,k} \):** This graph consists of \( k \) rows of hexagons with exactly \( n \) hexagons in each row with two extra edges. In the following \( Z_{9,5} \) is drawn:
It can be seen that the number of vertices $Z_{n,k}$ is equal to $|V(Z_{n,k})| = z_{n,k} = 2(n + 1)(k + 1)$.

$M_{n,k}$: This graph consists of $k$ rows of hexagons such that in the last row ($k$ th row) there are exactly $n$ hexagons with two extra edges. In the following we draw $M_{11,6}$.

The number of vertices of this graph is equal to: $m_{n,k} = (k + 1)(2n - k + 3)$

$A_n$: This graph consists of $n$ rows of hexagons such that in row $n$ there are exactly $n$ hexagons with three extra edges. In the following we draw $A_7$.

The number of vertices of the graphs is $a_n = (n + 2)^2$. 
$Z_{n,k,l}$: This graph consists of $k$ rows of hexagons such that in the first $l$ row with exactly $n$ hexagons, and from $l+1$ to $k$ th row the number of hexagons decrease by one in each row from its previous one. We draw $Z_{11,6,2}$ in the following

![Figure 5: The graph of $Z_{11,6,2}$.

The number of vertices of this graph is: $z_{n,k,l} = 2(n + 1)(k + 1) - (k - l + 1)^2$.

**Remark1.** For each of the graphs $(Z_{n,k}, M_{n,k}, A_n$ and $Z_{n,k,l})$, in the present figure for example for the graph $Z_{n,k,l}$, the edges lying on each line in the following figure is equivalent to one of $F_i$ in theorems 1 and 2. Moreover they constitute a partition on the set of edges. Also for other mentioned graph similar partition exists.

![Figure 6: Partition of Edges](image)

In figure 6 we have removed the set of edges lying on one of lines in figure 7, so by the remark 1 we have a two component graph with each component a convex subgraph of $Z_{n,k,l}$. For more explanation see [11] and [12].
Remark 2: In theorems 1 and 2 we can see that $E(G_1)$, $E(G_2)$ and $F_i$ partition $E(G)$ and $V(G_1)$ and $V(G_2)$ partition $V(G)$ for each $i$.

Lemma 1. we have

$$W(A_n) = 9 + \frac{261}{10} n + 29n^2 + \frac{31}{2} n^3 + 4n^4 + \frac{2}{5} n^5$$

Proof: If in $A_n$ we delete a collection of edges that seem to be parallel in one row according to remark 1, then $A_n$ is partitioned into two subgraphs of the form $A_r$ and $M_{st}$. Therefore there is a partition of edges of the graph satisfying Theorem 2. Hence by Theorem 2 we can write

$$W(A_n) = \sum_{i=1}^{n} |V(G_1)| |V(G_2)| = \sum_{i=0}^{n} (a_{i-1} \times m_{n,n-i})$$

$$= 9 + \frac{261}{10} n + 29n^2 + \frac{31}{2} n^3 + 4n^4 + \frac{2}{5} n^5$$

Lemma 2: we have

$$W(Z_{n,k}) = 1 + \frac{56}{15} k + \frac{32}{3} nk + \frac{11}{3} n + 4k^2 + \frac{1}{3} nk^4 + 6n^2k^2 + \frac{2}{3} n^2k^3 - \frac{1}{15} k^5 + \frac{4}{3} n^3 + \frac{4}{3} n^3k^2 + \frac{8}{3} n^3k + \frac{28}{3} nk^2 + \frac{5}{3} nk^3 + 4n^2 + \frac{4}{3} k^3 + \frac{28}{3} n^2k$$

Proof. By referring to the graph of $Z_{n,k}$ we observe that the set of edges that seem to be parallel forms a partition of $E(Z_{n,k})$ and if we delete these edges we obtain a graph with two connected components which are convex subgraphs. Now using Theorems 2 and the fact that $V(G) = V(G_1) \cup V(G_2)$, $1 \leq i \leq k$, and one of the components is a graph of type $A_r$, we can write:

$$W(Z_{n,k}) = 2 \sum_{i=1}^{k} a_{i-1} \cdot (z_{n,k} - a_{i-1}) + \sum_{i=0}^{n-k-2} m_{k+i,k} \cdot (z_{n,k} - m_{k+i,k})$$
Now by Theorem 1, if the graph detail of the calculation is as follows:

\[
W(M_{n,k}) = 2 \sum_{i=0}^{k} a_{i-1} \cdot (m_{n,k} - a_{i-1}) + \sum_{i=0}^{n-k-1} m_{k+i,k} \cdot (m_{n,k} - m_{k+i,k})
\]

\[
= 4 + \frac{26}{3} n + \frac{109}{15} k + \frac{5}{2} k^2 + 16 n k + 4 n k^2 - \frac{2}{3} k^3 n - \frac{5}{2} k^3 + \frac{34}{3} n^2 k + 6 n^2 + \frac{2}{3} n k^4 + \frac{8}{3} n^3 k + 4 n^2 k^2 - \frac{4}{3} n^3 k^2 - \frac{2}{3} n^2 k - \frac{4}{3} n^3 k^2 - \frac{4}{15} k^5 - \frac{4}{3} n^3 k^2
\]

Next we compute the Wiener index of the graph \(M_{n,k}\). But this is done using the same method as above and the calculation is as follows:

\[
W(Z_{n,k,l}) = \sum_{i=0}^{k} a_{i-1} \cdot (z_{n,k,l} - a_{i-1}) + \sum_{i=0}^{n-k-1} m_{k+i,k} \cdot (z_{n,k,l} - m_{k+i,k})
\]

\[
= \frac{4}{5} l + \frac{2}{3} k + \frac{2}{3} n + \frac{4}{3} n k - \frac{5}{6} k^2 + \frac{13}{3} l n + \frac{4}{3} k l + \frac{3}{2} l^2 - \frac{1}{6} k^2 l + \frac{23}{6} k l^2 + 2 k^2 l^2 - \frac{7}{6} k^3 - \frac{2}{3} k^4 + 7 k l n + 4 l^2 n k - \frac{4}{3} l^2 n k + \frac{1}{3} l^2 n + \frac{1}{3} n^2 k + 2 n^2 - \frac{7}{6} l^3 n - 2 l^2 n^2 + 4 l n^2 + 8 l n^2 k + 4 k^2 l n + 4 k^2 n^2 l - 2 n^2 l^2 k - \frac{4}{3} l^3 k + \frac{2}{3} n k^4 + \frac{2}{3} k^4 l - \frac{2}{3} k^4 l^2 - \frac{4}{3} k^3 n^2 + \frac{1}{3} k l^4 - \frac{4}{15} k^5 + \frac{4}{3} n^3 - \frac{2}{15} l^5 + \frac{4}{3} n^3 k^2 + \frac{2}{3} n^3 k - \frac{1}{3} l^4 n
\]

With the same method the Wiener index of the graph \(Z_{n,k,l}\) is computed in general. the detail of the calculation is as follows:

Now by Theorem 1, if the graph \(G\) has the appropriate property, then for the hyper-Wiener index of \(G\) we can write:

\[
WW(G) = \frac{n+1}{2} W(G) - \frac{1}{2} \sum_{i=1}^{n} (W(G^1_i) + W(G^2_i))
\]

Therefore to find the hyper-Wiener index of \(G\) one has to find the Wiener index of the subgraphs \(G^1_i\) and \(G^2_i\) instead of \(|V(G^2_i)|\) and \(|V(G^2_i)|\) and the Wiener index of \(G\), but \(G^1_i\)
and $G_2^I$ are isomorph to the graphs $Z_{n,k}$ or $M_{n,k}$ or $A_n$ of $Z_{n,k,l}$. Therefore by our previous Computation one can see that:

$$WW(Z_{n,k}) = (n + k + 1)W(Z_{n,k})$$

$$= \frac{1}{2} \left[ n \sum_{i=0}^{k-1} 2 \left( W(A_{i-1}) + W(Z_{n,k,i-1}) \right) + \sum_{i=1}^{n-k-2} \left( W(M_{k+i,k}) + W(M_{n-2-i,k}) \right) + 2 \left( W(A_{k-1}) + W(M_{n-1,k}) \right) + \sum_{i=1}^{n-1} \left( W(Z_{n,k-i}) + W(Z_{n,i-1}) \right) + \sum_{i=1}^{n} \left( W(Z_{n,i}) + W(Z_{i-1}) \right) \right]$$

$$= 1 + \frac{43}{10} k + \frac{21}{5} n + \frac{211}{36} k^2 + \frac{1043}{180} n^2 + \frac{1283}{90} nk + \frac{2}{3} n^2 k^2 + \frac{10}{3} k^3 n^2$$

$$+ \frac{3}{3} k^2 n^3 + \frac{67}{9} k n^3 + \frac{1}{3} k^2 n^2 + \frac{67}{9} n k^3 + \frac{47}{3} k^3 n^2 - \frac{2 \cdot 15}{15} k^5 + \frac{10}{3} n^3 + \frac{10}{3} k^3$$

$$+ \frac{2}{5} k n^4 + \frac{25}{36} k^4 + \frac{1}{2} k^4 n^2 + \frac{1}{2} k^5 n^2 + \frac{38}{3} n^2 k^2 + \frac{2 \cdot 10}{18} k^6$$

$$+ \frac{5}{6} k^2 n^4 - \frac{1}{15} n^5 k + \frac{1}{90} n^6$$

And similarly:

$$WW(M_{n,k})$$

$$= \left( \frac{2n + k + 3}{2} \right) W(M_{n,k})$$

$$= \frac{1}{2} \left[ n \sum_{i=0}^{k-1} 2 \left( W(A_{i-1}) + W(Z_{n,k,i-1}) \right) + \sum_{i=1}^{n-k-1} 2 \left( W(Z_{k,i}) + W(M_{n-1-i,k}) \right) + 2 \left( W(A_{k-1}) + W(Z_{n-1,k}) \right) + \sum_{i=1}^{n} \left( W(M_{n-i,k-1}) + W(M_{n,i-1}) \right) \right]$$
As we mentioned earlier, our aim is to calculate the hyper-Wiener index of the graph $G_n$ which is the graph of one-pentagonal carbon nanocone. It consists of a pentagon as its center and is surrounded by $n$ layers of hexagons. The graph of $G_n$ can be seen in section 2. In this section using previous results we reach to our goal.

For a general graph $G$ and a subset $F \subseteq V(G)$ let us define $(F)_G$ as the induced or generated subgraph by $F$ whose vertex set is $F$ and the edge set is:

$$E((F)_G) = \{uv = e \in E(G) \mid u, v \in F\}$$

Now consider the graph of $G_n$ and partition it in five sets $F_i$, $1 \leq i \leq 5$. For simplicity we show these partitions for $G_6$ as follows:

![Figure 8: Partitions of $G_6$](image)

We can see that

$$(F_1)_{G_n} \ll G_n$$

$$(F_1 \cup F_2)_{G_n} \ll G_n$$

3. Computation with one-pentagonal Carbon nanocone.

$$= 5 + \frac{113}{12}k + \frac{193}{15}n + \frac{4}{3}k^2n^4 - \frac{2}{15}kn^5 - \frac{34}{15}nk^5 + \frac{727}{30}nk + \frac{35}{6}nk^2 - \frac{23}{6}k^3n$$

$$+ \frac{22}{3}n^2k - \frac{1}{3}nk^4 + \frac{26}{3}n^3k + \frac{41}{6}n^2k^2 - \frac{2}{3}k^3n^2 + \frac{2}{24}n^3k^2 + \frac{7}{24}k^4 + \frac{2123}{180}n^2$$

$$+ \frac{133}{120}k^2 - \frac{29}{12}k^3 + \frac{14}{3}n^3 + \frac{5}{3}n^4k + \frac{1}{90}n^6 + \frac{3}{5}k^6 + \frac{10}{3}k^4n^2 - \frac{8}{3}k^3n^3 - \frac{1}{30}n^5$$

$$+ \frac{25}{36}n^4$$
Now if we consider $G_n$, we see that
\[ (F_1)_{G_n} \equiv A_n \]
\[ (F_1 \cup F_2)_{G_n} \equiv Z_{n\times n} \]
\[ (F_1 \cup F_2 \cup F_3)_{G_n} \equiv M_{2n\times n} \]

Theorem 3. Let $Z_{n,k}$, $M_{n,k}$ and $G_n$ be the graphs that were mentioned previously. Then for any real number $\lambda$ we have:
\[ W_\lambda(G_n) = 5 \left( W_\lambda(M_{2n\times n}) - W_\lambda(Z_{n\times n}) \right) \]

Proof: we saw that $\{F_i\}_{i=1}^n$ is a partition of the vertex set of $G_n$. By definition 2 we can write:
\[ D^\lambda(F_1, G_n) = \sum_{i=1}^{5} D^\lambda_{G_n}(F_1, F_i) = D^\lambda_{G_n}(F_1, F_1) + 2D^\lambda_{G_n}(F_1, F_2) + 2D^\lambda_{G_n}(F_1, F_3) \]
And
\[ D^\lambda_{G_n}(F_1 \cup F_2, F_1 \cup F_2) = 2D^\lambda_{G_n}(F_1, F_1) + 2D^\lambda_{G_n}(F_1, F_2) \]
And
\[ D^\lambda_{G_n}(F_1 \cup F_2 \cup F_3, F_1 \cup F_2 \cup F_3) = 4D^\lambda_{G_n}(F_1, F_2) + 3D^\lambda_{G_n}(F_1, F_1) + 2D^\lambda_{G_n}(F_1, F_3) \]
Hence
\[ D^\lambda(F_1, G_n) = D^\lambda_{G_n}(F_1 \cup F_2 \cup F_3, F_1 \cup F_2 \cup F_3) - D^\lambda_{G_n}(F_1 \cup F_2, F_1 \cup F_2) \]

But we already seen:

\[ \langle F_1 \cup F_2 \cup F_3 \rangle_{G_n} \cong M_{2n,n}, \langle F_1 \cup F_2 \rangle_{G_n} \cong Z_{n,n} \]

And using the results

\[ D^\lambda(F_1 \cup F_2 \cup F_3, F_1 \cup F_2 \cup F_3) = 2W_\lambda(M_{2n,n}) \]

\[ D^\lambda(F_1 \cup F_2, F_1 \cup F_2) = 2W_\lambda(Z_{n,n}) \]

And finally

\[ D^\lambda(F_1, G_n) = W_\lambda(M_{2n,n}) - W_\lambda(Z_{n,n}) \]

Now using definition 2 we have

\[ W_\lambda(G_n) = \frac{1}{2} \sum_{i=1}^{5} \sum_{j=1}^{5} D^\lambda_{G_n}(F_i, F_j) = \frac{1}{2} \sum_{i=1}^{5} D^\lambda(F_i, G_n) = \frac{5}{2} D^\lambda(F_i, G_n) \quad 1 \leq i \leq 5 \]

So

\[ W_\lambda(G_n) = \frac{5}{2} D^\lambda(F_1, G_n) \]

And finally

\[ W_\lambda(G_n) = 5 \left( W_\lambda(M_{2n,n}) - W_\lambda(Z_{n,n}) \right) \]

**Theorem 4.** We have

\[ WW(G_n) = 20 + \frac{533}{4} n + \frac{8501}{24} n^2 + \frac{5795}{12} n^3 + \frac{8575}{24} n^4 + \frac{409}{3} n^5 + 21n^6 \]

Proof. Using theorem 3 and the following fact

\[ WW(G_n) = 5 \left( WW(M_{2n,n}) - WW(Z_{n,n}) \right) \]

Since we already calculated \( WW(M_{n,k}) \) and \( WW(Z_{n,k}) \), therefore we can calculate \( WW(M_{2n,n}) \) and \( WW(Z_{n,n}) \), as follows

\[ WW(Z_{n,n}) = 1 + \frac{17}{2} n + \frac{1166}{45} n^2 + 38n^3 + \frac{521}{18} n^4 + 11n^5 + \frac{74}{45} n^6 \]
\[ WW(M_{2n,n}) = 5 + \frac{703}{20} n + \frac{34831}{360} n^2 + \frac{1615}{12} n^3 + \frac{7229}{72} n^4 + \frac{574}{15} n^5 + \frac{263}{45} n^6 \]

Now using theorem 3 we finally obtain:

\[ WW(G_n) = 20 + \frac{533}{4} n + \frac{8501}{24} n^2 + \frac{5795}{12} n^3 + \frac{8575}{24} n^4 + \frac{409}{3} n^5 + 21 n^6 \]

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