The Hyper-Wiener Index of One-pentagonal Carbon Nanocone

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Abstract: One-pentagonal carbon nanocone consists of one pentagon as its core surrounded by layers of hexagons. If there are *n* layers, then the graph of the molecules is denoted by G_n. In this paper our aim is to explicitly calculate the hyper-Wiener index of G_n.

Keywords: Topological index, hyper-Wiener index, nanocone.

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 $W(G)=\sum_{\{u,v\}\subseteq V(G)} d_G(u,v)$. Wiener index applied to chemical graphs, the graphs of molecules, was first introduced by H. Wiener [1]. Wiener used this index only for acyclic molecules in a slightly different way. The definition of the Wiener index in terms of distances between vertices of a graph was given by Hosoya [2]. The Wiener index of graphs has been extensively studied in [3-11]. In [6] Darafsheh proposed a new method to calculate the Wiener index of a graph. A generalization of the concept of the Wiener index in recent studies is the hyper-Wiener index, which was introduced in [12] and since then studied in many research works [13-15]. In this paper our aim is to explicitly calculate the hyper-Wiener index of the one-pentagonal carbon nanocone. Some applications of graph theory and group theory in chemistry can be found in the literature [16-22].

First we describe the notation which will be kept throughout the paper. The hyper-wiener index of a graph G is defined as the following.

Definition 1. Let G be a simple connected graph with vertex set $V(G)$. For a real number λ, we have $W_\lambda(G)=\sum_{\{u,v\}\subseteq V(G)} d_G(u,v)^\lambda$. 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 $WW(G)=\frac{1}{2}\sum_{\{u,v\}\subseteq V(G)}\left((d_G(u,v)^2+d_G(u,v)\right)=\frac{1}{2}\left(W_2(G)+W_1(G)\right)$.

Definition 2. Let G be a simple connected graph with a vertex set $V(G)$. For $F,K\subseteq V(G)$ the following quantity is defined: ${D_G}^\lambda(F,K)=\sum_{u\in F}\sum_{v\in K} d_G(u,v)^\lambda$, where λ is a real number. If $K=V(G)$, then we set $D_G^\lambda\left(F,V(G)\right)=D^\lambda(F,G)$.

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 terminology if $H \ll G$, then it is evident that $D_H^\lambda\left(V(H),V(H)\right)=2W_\lambda(H)$. And if $\{V_k\}_{k=1}^n$ is a partition of $V(G)$, then $W_\lambda(G)=\frac{1}{2}\sum_{i=1}^n\sum_{j=1}^n D_G^\lambda\left(V_i,V_j\right)$.

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 $W_{\lambda+1}(G)=nW_\lambda(G)-\sum_{i=1}^n\left(W_\lambda\left(G_1^i\right)+W_\lambda\left(G_2^i\right)\right)$, where λ is a real number.

Proof. See [23].

Theorem 2. 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 the Wiener index of G is $W(G)=\sum_{i=1}^n\left|V\left(G_1^i\right)\right|\left|V\left(G_2^i\right)\right|$.

Proof. See [23].

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 consists of one pentagon surrounded by layers of hexagons. If there are n layers, then this graph is denoted by G_n. In Fig. (**1**) the graph of G_6 is drawn:

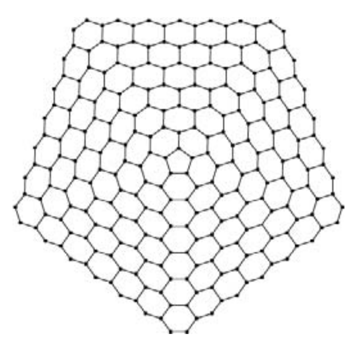

Fig. (1). The graph of G_6.

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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 graphs and draw them in special cases of n, k, and l.

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

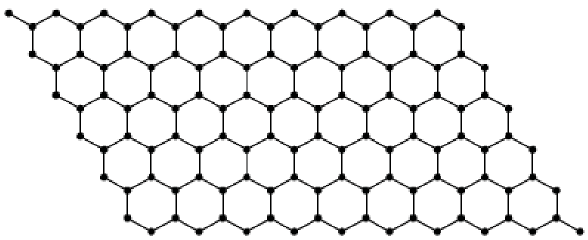

Fig. (2). The graph of $Z_{9,5}$.

$\boldsymbol{M_{n,k}}$ **:** 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 Fig. (**3**) we draw $M_{11,6}$. The number of vertices of this graph is equal to $m_{n,k} = (k+1)(2n-k+3)$.

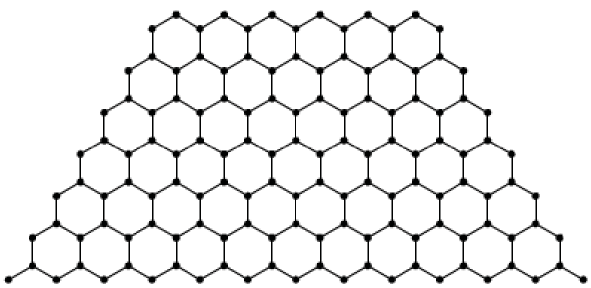

Fig. (3). The graph of $M_{11,6}$

$\boldsymbol{A_n}$ **:** This graph consists of n rows of hexagons such that in row n there are exactly n hexagons with three extra edges. In Fig. (**4**) we draw A_7. The number of vertices of the graphs is $a_n = (n+2)^2$.

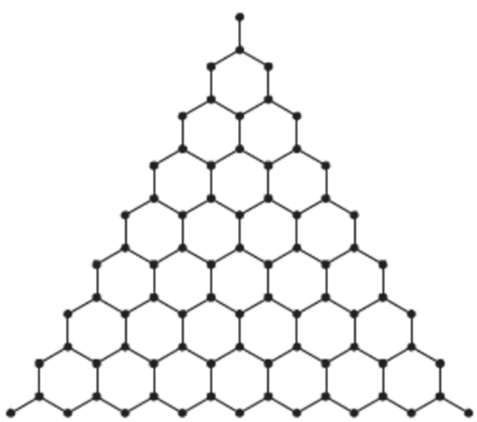

Fig. (4). The graph of A_7.

$\boldsymbol{Z_{n,k,l}}$ **:** This graph consists of k rows of hexagons such that in the first l row with exactly n hexagons, and from l+1-th 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 Fig. (**5**). The number of vertices of this graph is: $z_{n,k,l} = 2(n+1)(k+1) - (k-l+1)^2$.

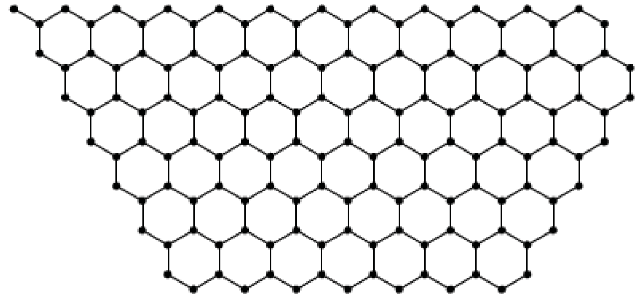

Fig. (5). The graph of $Z_{11,6,2}$.

Remark 1. 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.

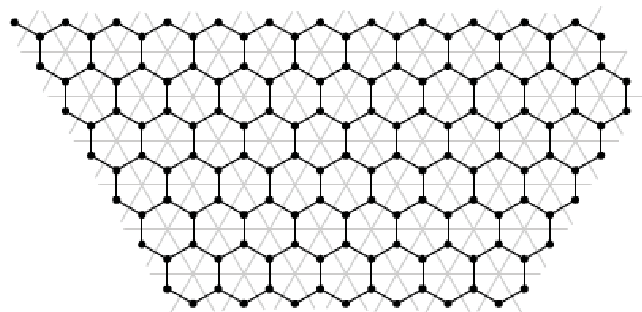

Fig. (6). Partition of Edges

In Fig. (**6**) we have removed the set of edges lying on one of the lines in Fig. (**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 [23].

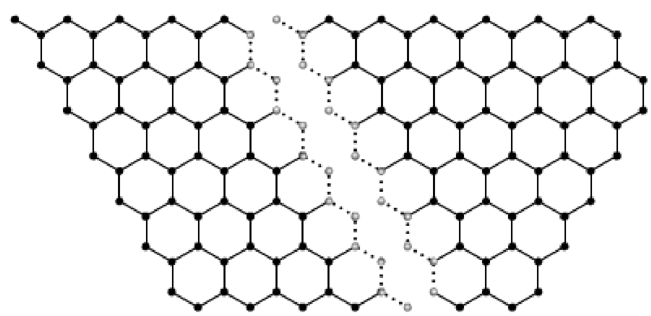

Fig. (7). Removing a set of edges from the graph.

Remark 2: In theorems 1 and 2 we can see that $E(G_1^i)$, $E(G_2^i)$, and F_i partition $E(G)$ and $V(G_1^i)$ and $V(G_2^i)$ 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 $M_{s,t}$. Therefore there is a partition of edges of the graph satisfying Theorem 2. Hence by Theorem 2 we can write $W(A_n) = \sum_{i=1}^{n} |V(G_1^i)||V(G_2^i)| = \sum_{i=0}^{n}(a_{i-1} \times m_{n,n-i}) = 9 + \frac{261}{10}n + 29n^2 + \frac{31}{2}n^3 + 4n^4 + \frac{2}{5}n^5$.

Lemma 2: we have

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

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 Theorem 2 and the fact that $V(G) = V(G_1^i) \cup V(G_2^i)$, $1 \le i \le k$, and one of the components is a graph of type A_r, we can write :

$$W(Z_{n,k}) = 2\sum_{i=1}^{k} a_{i-1}.(z_{n,k} - a_{i-1}) + \sum_{i=0}^{n-k-2} m_{k+i,k}.(z_{n,k} - m_{k+i,k}) + \sum_{i=1}^{n} z_{n-i,k}.(z_{n,k} - z_{n-i,k}) + \sum_{i=1}^{k} z_{n,k-i}.(z_{n,k} - z_{n,k-i}) = 1 + \frac{56}{15}k + \frac{32}{3}nk + \frac{11}{3}n + 4k^2 + \frac{1}{3}nk^4 + 6n^2k^2 + \frac{2}{3}n^2k^3 - \frac{1}{15}k^5 + \frac{4}{3}n^3 + \frac{4}{3}n^3k^2 + \frac{8}{3}n^3k + \frac{28}{3}nk^2 + \frac{8}{3}nk^3 + 4n^2 + \frac{4}{3}k^3 + \frac{28}{3}n^2k.$$

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:

$$W(M_{n,k}) = 2\sum_{i=0}^{k} a_{i-1}.(m_{n,k} - a_{i-1}) + \sum_{i=0}^{n-k-1} m_{k+i,k}.(m_{n,k} - m_{k+i,k}) + \sum_{i=1}^{k} m_{n-i,k-i}.(m_{n,k} - m_{n-i,k-i}) = 4 + \frac{26}{3}n + \frac{109}{15}k + \frac{1}{2}k^2 + 16nk + 4nk^2 - \frac{8}{3}k^3n - \frac{5}{2}k^3 + \frac{34}{3}n^2k + 6n^2 + \frac{2}{3}nk^4 + \frac{8}{3}n^3k + 4n^2k^2 - \frac{4}{3}k^3n^2 + \frac{4}{3}n^3k^2 - \frac{4}{15}k^5 + \frac{4}{3}n^3.$$

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:

$$W(Z_{n,k,l}) = \sum_{i=0}^{k} a_{i-1}.(z_{n,k,l} - a_{i-1}) + \sum_{i=0}^{n-k-2} m_{k+i,k}.(z_{n,k,l} - m_{k+i,k}) + \sum_{i=1}^{l} m_{k-i,l-i}.(z_{n,k,l} - m_{k-i,l-i}) + \sum_{i=1}^{k-l} z_{n,k-i,l}.(z_{n,k,l} - z_{n,k-i,l}) + \sum_{i=1}^{l} z_{n,l-i}.(z_{n,k,l} - z_{n,l-i}) + \sum_{i=0}^{n-k+l-1} z_{k,i}.(z_{n,k,l} - z_{k,i}) + \sum_{i=0}^{k-l-1} z_{n-k+l+i,k,k-i}.(z_{n,k,l} - z_{n-k+l+i,k,k-i}) = \frac{4}{5}l - \frac{1}{15}k + \frac{2}{3}n + \frac{4}{3}nk - \frac{5}{6}k^2 + \frac{13}{3}ln + \frac{4}{3}kl + \frac{3}{2}l^2 - \frac{1}{6}k^2l + \frac{23}{6}kl^2 + 2k^2l^2 - \frac{7}{6}k^3 - \frac{2}{3}k^4 + 7kln + 4l^2nk - \frac{4}{3}l^3nk + \frac{1}{3}l^2n + \frac{10}{3}n^2k + 2n^2 - \frac{7}{6}l^3 - \frac{4}{3}l^3n - 2l^2n^2 + 4ln^2 + 8ln^2k + 4k^2l^2n - \frac{8}{3}k^3ln + 4k^2n^2l - 2n^2l^2k - \frac{4}{3}l^3k + \frac{2}{3}nk^4 + \frac{2}{3}k^4l - \frac{2}{3}k^3l^2 - \frac{4}{3}k^3n^2 + \frac{1}{3}kl^4 - \frac{4}{15}k^5 + \frac{4}{3}n^3 - \frac{2}{15}l^5 + \frac{4}{3}n^3k^2 + \frac{8}{3}n^3k - \frac{1}{3}l^4n.$$

Now by Theorem 1, if the graph G has the appropriate property, then for the hyper-Wiener index of G we can write $WW(G) = \frac{n+1}{2}W(G) - \frac{1}{2}\sum_{i=1}^{n}\left(W(G_1^i) + W(G_2^i)\right)$.

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 isomorphic to the graphs $Z_{n,k}$ or $M_{n,k}$ or A_n or $Z_{n,k,l}$. Therefore by our previous Computation one can see that:

$$WW(Z_{n,k}) = (n+k+1)W(Z_{n,k}) - \frac{1}{2}\Big[\sum_{i=0}^{k} 2\left(W(A_{i-1}) + W(Z_{n,k,k-i})\right) + \sum_{i=0}^{n-k-2}\left(W(M_{k+i,k}) + W(M_{n-2-i,k})\right) + 2\left(W(A_{k-1}) + W(M_{n-1,k})\right) + \sum_{i=1}^{k}\left(W(Z_{n,k-i}) + W(Z_{n,i-1})\right) + \sum_{i=1}^{n}\left(W(Z_{k,n-i}) + W(Z_{k,i-1})\right)\Big] = 1 + \frac{43}{10}k + \frac{21}{5}n + \frac{211}{36}k^2 + \frac{1043}{180}n^2 + \frac{1283}{90}nk + 2nk^4 + \frac{38}{3}n^2k^2 + \frac{10}{3}k^3n^2 + \frac{13}{3}k^2n^3 + \frac{67}{9}kn^3 + \frac{47}{3}nk^2 + \frac{67}{9}nk^3 + \frac{47}{3}kn^2 - \frac{2}{15}k^5 + \frac{10}{3}n^3 + \frac{10}{3}k^3 + \frac{3}{2}kn^4 + \frac{25}{36}k^4 + \frac{1}{2}k^4n^2 + \frac{1}{5}k^5n + \frac{2}{9}k^3n^3 - \frac{1}{30}n^5 + \frac{25}{36}n^4 - \frac{1}{18}k^6 + \frac{5}{6}k^2n^4 - \frac{1}{15}n^5k + \frac{1}{90}n^6.$$

And similarly:

$$WW(M_{n,k}) = \frac{(2n+k+3)}{2}W(M_{n,k}) - \frac{1}{2}\Big[\sum_{i=0}^{k-1} 2\left(W(A_{i-1}) + W(Z_{n-i,k,i+1})\right) + \sum_{i=0}^{n-k-1} 2\left(W(Z_{k,i}) + W(M_{n-i-1,k})\right) + 2\left(W(A_{k-1}) + W(Z_{n-k,k})\right) + \sum_{i=1}^{k}\left(W(M_{n-i,k-i}) + W(M_{n,i-1})\right)\Big] = 5 + \frac{113}{12}k + \frac{193}{15}n + \frac{4}{3}k^2n^4 - \frac{2}{15}kn^5 - \frac{34}{15}nk^5 + \frac{727}{30}nk + \frac{35}{6}nk^2 - \frac{23}{6}k^3n + 22n^2k - \frac{1}{3}nk^4 + \frac{26}{3}n^3k + \frac{41}{6}n^2k^2 - \frac{2}{3}k^3n^2 + 2n^3k^2 + \frac{7}{24}k^4 + \frac{2123}{180}n^2 + \frac{133}{120}k^2 - \frac{29}{12}k^3 + \frac{14}{3}n^3 + \frac{5}{3}n^4k + \frac{1}{90}n^6 + \frac{3}{5}k^6 + \frac{10}{3}k^4n^2 - \frac{8}{3}k^3n^3 - \frac{1}{30}n^5 + \frac{25}{36}n^4.$$

3. COMPUTATION WITH ONE-PENTAGONAL CARBON NANOCONE.

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 $\langle F \rangle_G$ as the induced or generated subgraph by F whose vertex set is F and the edge set is $E(\langle F \rangle_G) = \{uv = e \in E(G) \mid u, v \in F\}$.

Now consider the graph of G_n and partition it in five sets F_i, $1 \le i \le 5$. For simplicity we show these partitions for G_6 as follows (Fig. **8**):

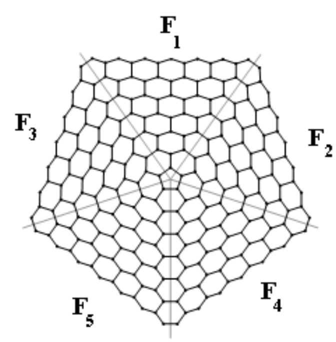

Fig. (8). Partitions of G_6

We can see that $\langle F_1 \rangle_{G_n} \ll G_n$, $\langle F_1 \cup F_2 \rangle_{G_n} \ll G_n$, and $\langle F_1 \cup F_2 \cup F_3 \rangle_{G_n} \ll G_n$. We will draw these graphs for the special case of G_6 (Fig. **9-11**):

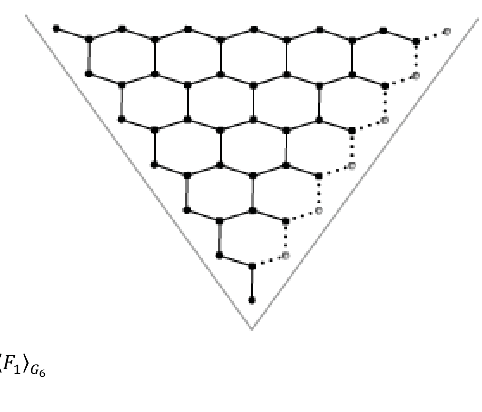

Fig. (9). $\langle F_1 \rangle_{G_6}$

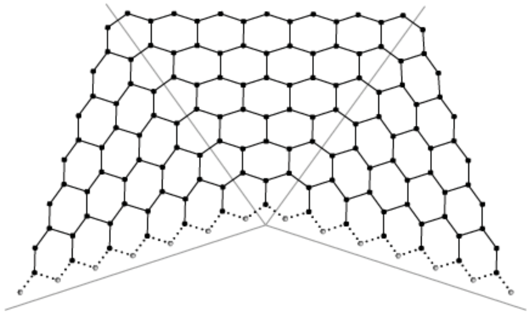

Fig. (10). $\langle F_1 \cup F_2 \rangle_{G_6}$

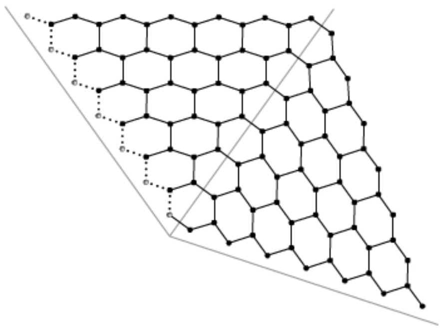

Fig. (11). $\langle F_1 \cup F_2 \cup F_3 \rangle_{G_6}$

Now if we consider G_n, we see that $\langle F_1 \rangle_{G_n} \cong A_n$, $\langle F_1 \cup F_2 \rangle_{G_n} \cong Z_{n,n}$, and $\langle F_1 \cup F_2 \cup F_3 \rangle_{G_n} \cong M_{2n,n}$.

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

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 the following equalities: $D^\lambda(F_1, G_n) = \sum_{i=1}^{5} D_{G_n}^\lambda(F_1, F_i) = D_{G_n}^\lambda(F_1, F_1) + 2D_{G_n}^\lambda(F_1, F_2) + 2D_{G_n}^\lambda(F_1, F_3)$. And

$D_{G_n}^\lambda(F_1 \cup F_2, F_1 \cup F_2) = 2D_{G_n}^\lambda(F_1, F_1) + 2D_{G_n}^\lambda(F_1, F_2)$. And

$D_{G_n}^\lambda(F_1 \cup F_2 \cup F_3, F_1 \cup F_2 \cup F_3) = 4D_{G_n}^\lambda(F_1, F_2) + 3D_{G_n}^\lambda(F_1, F_1) + 2D_{G_n}^\lambda(F_1, F_3)$. Hence

$D^\lambda(F_1, G_n) = D_{G_n}^\lambda(F_1 \cup F_2 \cup F_3, F_1 \cup F_2 \cup F_3) - D_{G_n}^\lambda(F_1 \cup F_2, F_1 \cup F_2)$. But we already saw:

$\langle F_1 \cup F_2 \cup F_3 \rangle_{G_n} \cong M_{2n,n}$ and $\langle F_1 \cup F_2 \rangle_{G_n} \cong Z_{n,n}$. And using the results $D^\lambda(F_1 \cup F_2 \cup F_3, F_1 \cup F_2 \cup F_3) = 2W_\lambda(M_{2n,n})$ and $D^\lambda(F_1 \cup F_2, F_1 \cup F_2) = 2W_\lambda(Z_{n,n})$, And finally $D^\lambda(F_1, G_n) = W_\lambda(M_{2n,n}) - W_\lambda(Z_{n,n})$. Now using Definition 2 we have $W_\lambda(G_n) = \frac{1}{2}\sum_{i=1}^{5}\sum_{j=1}^{5} D_{G_n}^\lambda(F_i, F_j) = \frac{1}{2}\sum_{i=1}^{5} D^\lambda(F_i, G_n) = \frac{5}{2} D^\lambda(F_i, G_n)$ $1 \le i \le 5$, 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: $WW(Z_{n,n}) = 1 + \frac{17}{2}n + \frac{1166}{45}n^2 + 38n^3 + \frac{521}{18}n^4 + 11n^5 + \frac{74}{45}n^6$, and $WW(M_{2n,n}) = 5 + \frac{703}{20}n + \frac{34831}{360}n^2 + \frac{1615}{12}n^3 + \frac{7229}{72}n^4 + \frac{574}{15}n^5 + \frac{263}{45}n^6$. Now using Theorem 3 we finally obtain: $WW(G_n) = 20 + \frac{533}{4}n + \frac{8501}{24}n^2 + \frac{5795}{12}n^3 + \frac{8575}{24}n^4 + \frac{409}{3}n^5 + 21n^6$.

CONFLICT OF INTEREST

The authors confirm that this article content has no conflicts of interest.

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