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Dedicated to Professor Mircea Diudea on the Occasion of His 65th Anniversary

POLYHEDRAL GRAPHS UNDER AUTOMORPHISM GROUPS

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ABSTRACT. A modified Wiener number was proposed by Graovać and Pisanski. It is based on the full automorphism group of a graph. In this paper, we compute the difference between these topological indices for some polyhedral graphs.

Keywords: *automorphism, polyhedral graphs, topological indices.*

INTRODUCTION

A topological index is a numerical value associated to a chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. In an exact phrase, if $\sum$ denotes the class of all finite graphs then a topological index is a function Top from $\sum$ into real numbers with the property that Top(Γ_1) = Top(Γ_2), if the graphs Γ_1 and Γ_2 are isomorphic. Obviously, the number of vertices and the number of edges may be considered as topological indices. Wiener index is the first reported distance based topological index defined as half sum of the distances between all the pairs of vertices in a molecular graph. Topological indices are abundantly used in QSPR and QSAR researches. So far, a variety of topological indices have been described. The Wiener number is one of them. It is the first reported distance based topological index. The Wiener number is defined as the half sum of distances between all the pairs of vertices in a molecular graph [1]. Randić defined the hyper–Wiener index

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of acyclic graphs [2], and then Klein et al. [3] generalized Randić's definition for all connected graphs, as a generalization of the Wiener index. It is defined as:

$$WW(\Gamma) = 1/2W(\Gamma) + 1/2\sum_{\{x,y\}}(d(x,y))^2. \tag{1}$$

We refer to [4-6] for mathematical properties and chemical meaning of this topological index.

An automorphism of the graph Γ is a bijection α on it, which preserves the edge set E *i.e.*, if $e=uv$ is an edge, then $\alpha(e)= \alpha(u)\alpha(v)$ is an edge of E. Here the image of vertex u is denoted by $\alpha(u)$. We denote the set of all automorphisms of Γ by Aut(Γ) and this set, under the composition of mappings, forms a group. This group acts transitively on the set of vertices, if for any pair of vertices $u,v \in V$, there is an automorphism α such that $\alpha(u)=v$.

By means of automorphism group, Graovać and Pisanski proposed the modified Wiener index [7,8], as follows:

$$\hat{W}(\Gamma) = \frac{|V(\Gamma)|}{2|G|}\sum_{x\in V(\Gamma)}\sum_{\alpha\in G} d(x,\alpha(x)), \tag{2}$$

In [9], a modified hyper–Wiener index was defined as:

$$\hat{WW}(\Gamma) = \frac{1}{2}\hat{W}(\Gamma) + \frac{|V(\Gamma)|}{4|G|}\sum_{u\in V(\Gamma),\alpha\in G} d(u,\alpha(u))^2. \tag{3}$$

Theorem 1 [7]**.** Let Γ be a graph with automorphism group G = Aut(Γ) and the vertex set $V(\Gamma)$. Let V_1, V_2, …, V_k be all orbits of action of G on $V(\Gamma)$. Then

$$\hat{W}(\Gamma) = |V(\Gamma)|\sum_{i=1}^{k}\frac{W(V_i)}{|V_i|}. \tag{4}$$

Corollary 2. Let Γ be a vertex-transitive graph, then $W(\Gamma) = \hat{W}(\Gamma)$.

It is easy to see that the Wiener index is equal to the modified Wiener index if Γ is vertex-transitive and the modified Wiener index is zero if and only if Aut(Γ) is trivial. For a given graph Γ, the difference between Wiener and modified Wiener indices is [10,11]:

$$\delta(\Gamma) = W(\Gamma) - \hat{W}(\Gamma). \tag{5}$$

Similarly, the difference between hyper–Wiener and modified hyper–Wiener indices can be written as:

$$\delta\delta(\Gamma) = WW(\Gamma) - \hat{WW}(\Gamma). \tag{6}$$

Example 3 [8]**.** Wiener index of Circumcoronenes with $5n^2$ vertices, for $n \geq 2$ is:

$$W(C_{5n^2}) = \frac{1}{6}(124n^5 - 35n^3 + n),$$

and the modified-Wiener index of circumcoronenes for $n \geq 2$ is:

$$\hat{W}(C_{5n^2}) = \frac{1}{3}n^3(n^2 - 10).$$

Then, we have

$$\delta(C_{5n^2}) = \frac{n}{6}(14n^4 - 15n^2 + 1).$$

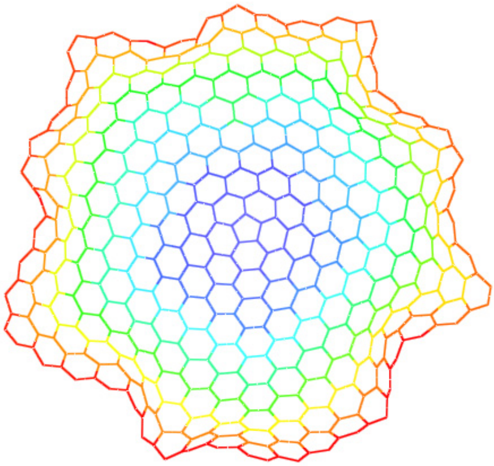

Figure 1. Circumcoronene; n=9.

Example 4 [8]**.** Wiener index of circumcoronenes with $6n^2$ vertices, for $n \geq 1$, is:

$$W(C_{6n^2}) = \frac{n}{5}(164n^4 - 30n^2 + 1)$$

and the modified-Wiener index of circumcoronenes for $n \geq 1$ is:

$$\hat{W}(C_{6n^2}) = 30n^5 - 3n^3.$$

Hence, we can deduce that

$$\delta(C_{6n^2}) = \frac{n}{5}(14n^4 - 15n^2 + 1).$$

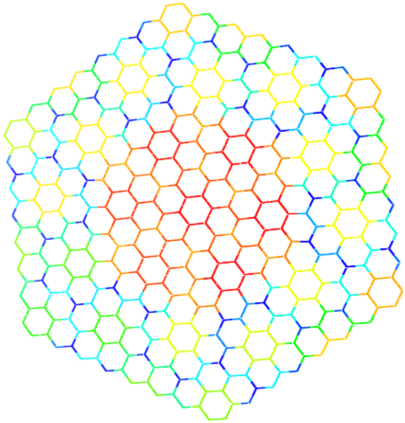

Figure 2. Circumcoronene; n=8.

RESULTS AND DISCUSSION

A planar graph is the one that can be drawn on the plane in such a way that its edges intersect only at their endpoints. Let Γ be a planar graph and n, m, f are respectively the number of vertices, edges and faces. Then by Euler theorem, we have

$$n - m + f = 2 \tag{7}$$

A general polyhedron is the one that satisfies the Euler relation. If a cubic polyhedron has no face of size greater than 6, then it has a positive curvature. In [12], Ghorbani introduced a new class of fullerene graphs with pentagons and heptagons. In this paper, we also introduce a class of polyhedral graphs with squares, pentagons and hexagons (Figures 3;4).

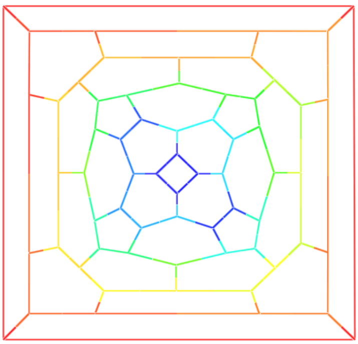

Figure 3. The Case of n = 4 in C_{16n}.

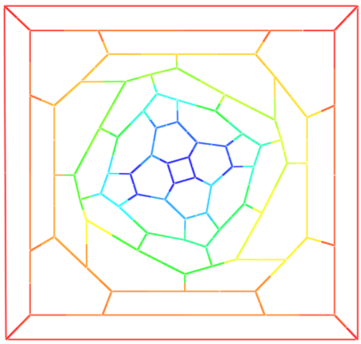

Figure 4. The Case of n = 5 in C_{16n}.

This class of polyhedral graphs has exactly 16*n* vertices, where *n* is an integer greater than or equal with 4, herein denoted by C_{16n}. By Euler's formula, we can conclude that this graph has exactly 2 squares, 8 pentagons and 8(*n*-1) hexagons*, for* $n \geq 4$.

Theorem 5. For $n \geq 4$*,* the automorphism group of graph C_{16n} is isomorphic to

$$Aut(C_{16n}) \cong \begin{cases} D_{16} & n \mid 2 \\ D_8 & n \nmid 2 \end{cases}.$$

Proof. At first we compute the order of $G = Aut(C_{16n})$ of symmetries of the polyhedral graph C_{16n}, for *n*=4 depicted in Figure 5; the automorphism group of C_{16n} for $n \geq 5$ and *n*|2 can be computed similarly. If α denotes the rotation of C_{16n} for 45° and β is a reflection over the central vertical line, then $G \geq \prec \alpha, \beta \succ$. On the other hand, $|\prec \alpha, \beta \succ| = 16$ where $\alpha^8 = \beta^2 = 1$, $\beta\alpha\beta = \alpha^{-1}$. This leads us to conclude that $G = \prec \alpha, \beta \succ \cong D_{16}$.

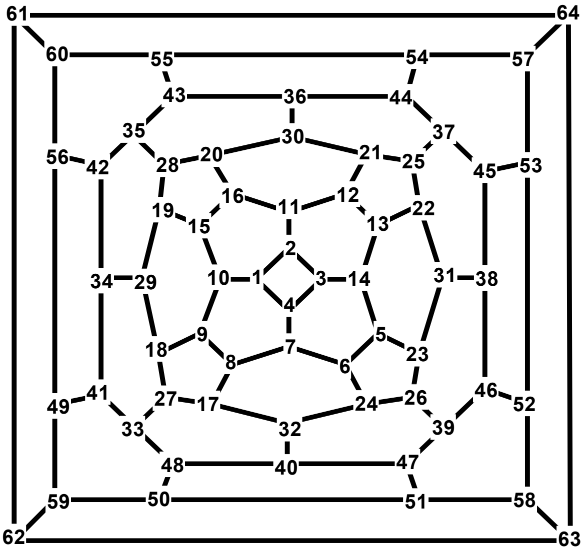

Figure 5. Labeling of cubic polyhedral graph C_{16n} for *n*=4.

Similarly, for $n \nmid 2$, $G \cong D_8$ and the proof is completed.

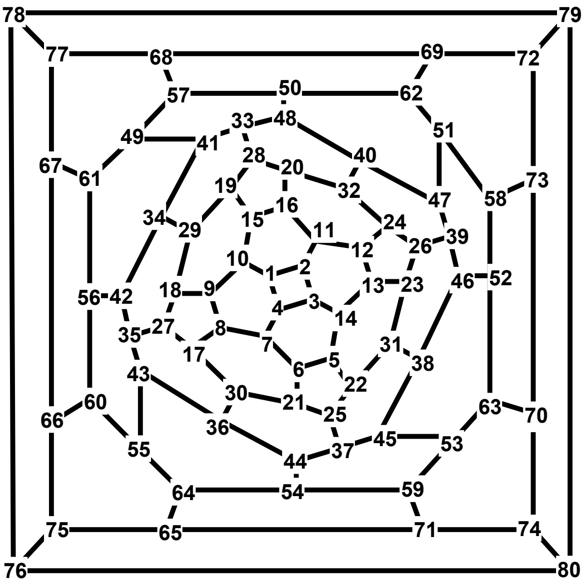

Figure 6. Labeling of cubic polyhedral graph C_{16n} for *n*=5.

Now, we prove that the Wiener index of this class of polyhedral graphs for $n \geq 9$ is:

$$W(C_{16n}) = \frac{256}{3}n^3 + \frac{8384}{3}n - 7432. \qquad (8)$$

The Wiener index of this class of polyhedral graphs is computed for the first time in this paper. We can also apply our method to compute the other classes of polyhedral graphs. In [13], a method to obtain a polyhedral graphs from a zig – zag or armchair nanotubes, is described. Here, by continuing this method, we can construct an infinite class of polyhedral graphs and then compute its Wiener number. The symbol $T_Z[m,n]$ means a zig–zag nanotube with *m* rows and *n* columns of hexagons (see Figure 7). Combine a nanotube $T_Z[8,n]$ with two copies of cap *B* (Figure 8) as shown in Figure 9; the resulted graph is a polyhedral graph with 16*n* vertices, for $n \geq 9$.

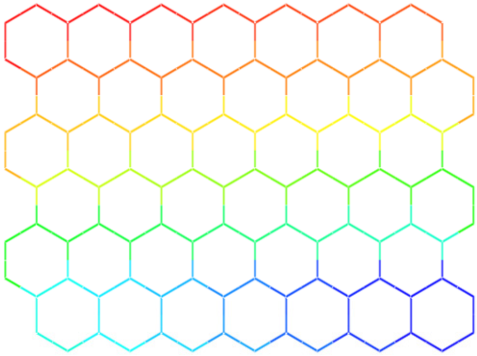

Figure 7. $2D$ graph of a zig–zag nanotube $T_Z[m,n]$, for $m = 8$; $n = 6$.

A block matrix can be written in terms of smaller matrices. In the following theorem, the Wiener index of the $G = T_Z[8,n]$ nanotube for $n \geq 9$ is computed, see Figure 9.

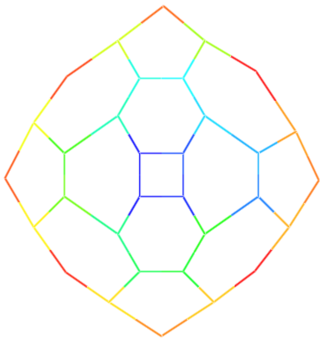

Figure 8. Cap *B.*

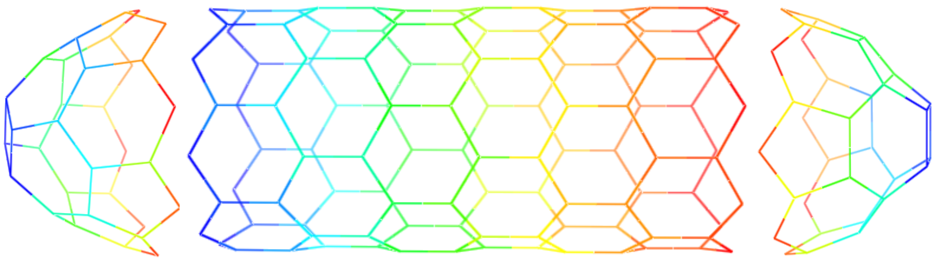

Figure 9. Polyhedral graph C_{16n} constructed by combining two copies of cap *B,* and the zig-zag nanotube $T_Z[8,n]$.

Theorem 6. For $n \geq 9$,

$$W(T_Z[8,n]) = \frac{256}{3}n^3 - 512n^2 + \frac{11072}{3}n - 11392. \qquad (9)$$

Proof. According to Figure 9, there are $n + 1$ rows of vertices. We suppose the vertices of the last row are $U = \{u_1, u_2, \ldots, u_{16}\}$. To compute the Wiener index of this nanotube we use a recursive sequence method. Let t_n be the two times of Wiener index of $G = T_Z[8, n]$. A straightforward computation yields the recurrence

$$\begin{aligned} 2W(G) = t_n &= \sum_{x,y\in U} d(x,y) + \sum_{x,y\in V\setminus U} d(x,y) + 2\sum_{x\in U, y\in V\setminus U} d(x,y) \\ &= 1024 + t_{n-1} + 2\sum_{x\in U, y\in V\setminus U} d(x,y). \end{aligned} \qquad (10)$$

To compute the summation $\sum_{x\in V, y\in V\setminus U} d(x,y)$ by using the symmetry of graph we have

$$\sum_{x\in U, y\in V\setminus U} d(x,y) = 8(d(u_1) + d(u_2)), \qquad (11)$$

where $d(u_1) = \sum_{y\in V\setminus U} d(u_1, y)$ and $d(u_2)$ defines the similarly (see Figure 10). By computing these values, one can see that:

$$\begin{aligned} d(u_1) &= 16n^2 - 72n + 184, \quad n \geq 9, \\ d(u_2) &= 16n^2 - 88n + 288, \quad n \geq 10. \end{aligned} \qquad (12)$$

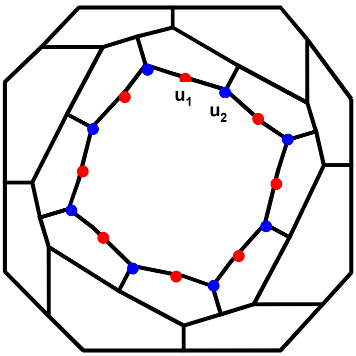

Figure 10. 2-D graph of the nanotube $T_Z[8,2]$.

This implies that t_{n+1} = $1024 + t_n + 8(d(u_1) + d(u_2))$. The solution of this recurrence is

$$W(G) = \frac{256}{3}n^3 - 512n^2 + \frac{11072}{3}n - 11392. \qquad (13)$$

Theorem 7. For $n \geq 9$**,**

$$W(C_{16n}) = \frac{256}{3}n^3 + \frac{8384}{3}n - 7432. \qquad (14)$$

Proof. From Figure 9, one can see that the distance matrix of polyhedral graph C_{16n} can be written as a block matrix as follows:

Suppose $\{v_1, v_2, \ldots, v_r\}$, $\{u_1, \ldots, u_s\}$ and $\{w_1, \ldots, w_r\}$ be the set of vertices of the first cap, vertices of $T_Z[8,n]$ and vertices of the second cap, respectively. The distance matrix D can be broken to the following form:

$$D = \begin{bmatrix} V & B & W \\ B & U & B \\ W & B & V \end{bmatrix},$$

where V, B and W are distances between vertices of the first cap with the vertices of $T_Z[8,n]$ and vertices of the second cap. The matrix U is the distance matrix of vertices $\{u_1, \ldots, u_s\}$. In other words, U is the distance matrix of $T_Z[8,n]$. This matrix was computed in Theorem 6. It is easy to see that the Wiener index is equal to the half-sum of distances of the distance matrix D between all pairs of vertices. For any polyhedral graph C_{16n} the matrix V is constant, as shown in Figure 11. The summation of entries of matrix V is 3880. Obviously, the distance matrices B, U and W are dependant to the number of rows in the nanotube $T_Z[8,n]$. In other words, if w_n and w_{n-1} be the Wiener indices of the polyhedral graphs C_{16n} and $C_{16(n-1)}$, respectively, then similar to the proof of the Theorem 1, for $n \geq 10$, we have

$w_{10} - w_9 = 25920$, $w_{11} - w_{10} = 31040$, $w_{12} - w_{11} = 36672$, $w_{13} - w_{12} = 42816$.

Again, a straightforward computation yields the recurrence

$$w_n - w_{n-1} = 256n^2 - 256n + 2880. \qquad (15)$$

and the solution of this recurrence is

$$W(C_{16n}) = \frac{256}{3}n^3 + \frac{8384}{3}n - 7432. \qquad (16)$$

This completes the proof.

Corollary 8. For polyhedral graph C_{16n}, we have

$$\delta(C_{16n}) = \begin{cases} \frac{64}{3}n^3 - 256n^2 + \frac{6704}{3}n - 7432, & n = 4k, k \geq 3 \\ \frac{64}{3}n^3 - 256n^2 + \frac{6896}{3}n - 7432, & otherwise \end{cases}, \tag{17}$$

$$\hat{\delta}\delta(C_{16n}) = \begin{cases} \frac{32}{3}n^3 - 864n^2 + \frac{41800}{3}n - 60524, & 2 \mid n,\ n = 4k, \\ \frac{32}{3}n^3 - 864n^2 + \frac{43432}{3}n - 60524,, & 2 \mid n,\ n = 2(2k-1). \\ \frac{32}{3}n^3 - 896n^2 + \frac{43144}{3}n - 60524, & 2 \nmid n \end{cases} \tag{18}$$

Proof. At first by a direct computation, we have

$$W(C_{64}) = 9984, W(C_{80}) = 17520, W(C_{96}) = 27864, W(C_{112}) = 41436, W(C_{128}) = 58624,$$

$$WW(C_{64}) = 34100,\ WW(C_{80}) = 65976,\ WW(C_{96}) = 114684,\ WW(C_{112}) = 185496,$$
$$WW(C_{128}) = 283916,\ WW(C_{144}) = 417748.$$

By applying the methods of [6], we have:

$$\begin{aligned} W(C_{16n}) &= \frac{256}{3}n^3 + \frac{8384}{3}n - 7432, \quad n \geq 9 \\ WW(C_{16n}) &= \frac{128}{3}n^4 + \frac{128}{3}n^3 + \frac{352}{3}n^2 + \frac{52576}{3}n - 60524, \quad n \geq 10. \end{aligned} \tag{19}$$

On the other hand, by using Theorem 5, we have:

$$\hat{W}(C_{64}) = 9760, \hat{W}(C_{80}) = 16480, \hat{W}(C_{96}) = 25824, \hat{W}(C_{112}) = 37912, \hat{W}(C_{128}) = 53568,$$

$$W\hat{W}(C_{64}) = 36128,\ W\hat{W}(C_{80}) = 67280,\ W\hat{W}(C_{96}) = 113568,$$
$$W\hat{W}(C_{112}) = 184352, W\hat{W}(C_{128}) = 281728.$$

and for $n \geq 9$, $k \geq 3$ we have:

$$\hat{W}(C_{16n}) = \begin{cases} 64n^3 + 256n^2 + 560n, & n = 4k \\ 64n^3 + 256n^2 + 496n, & otherwise \end{cases},$$

$$\widehat{WW}(C_{16n}) = \begin{cases} \dfrac{128}{3}n^4 + 32n^3 + \dfrac{2944}{3}n^2 + 3592n, & 2 \mid n,\ \ n = 4k, \\ \dfrac{128}{3}n^4 + 32n^3 + \dfrac{2944}{3}n^2 + 3048n, & 2 \mid n,\ \ n = 2(2k-1). \\ \dfrac{128}{3}n^4 + 32n^3 + \dfrac{3040}{3}n^2 + 3144n, & 2 \nmid n \end{cases} \qquad (20)$$

The proof can be drawn from (19) and (20).

$$V = \begin{bmatrix}
0, 1, 2, 1, 4, 3, 2, 3, 2, 1, 2, 3, 4, 3, 2, 3, 4, 3, 3, 4, 4, 5, 5, 4, 5, 5, 4, 4, 4, 5, 6, 5 \\
1, 0, 1, 2, 3, 4, 3, 4, 3, 2, 1, 2, 3, 2, 3, 2, 5, 4, 4, 3, 3, 4, 4, 5, 4, 5, 5, 4, 5, 4, 5, 6 \\
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\end{bmatrix}$$

Figure 11. Matrix $V(C_{16,n})$

CONCLUSION

In this paper, a new family of cubic polyhedral graphs was introduced and then its modified Wiener index was computed. Also, their Wiener index was computed and, finally, the difference between two topological indices was derived.

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