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ON THE GRAOVAC-PISANSKI INDEX

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ABSTRACT. The Graovac-Pisanski index (*GP* index) is an algebraic approach for generalizing the Wiener index. In this paper, we compute the difference between the Wiener and *GP* indices for an infinite family of polyhedral graphs.

Key words: Wiener index, polyhedral graphs.

INTRODUCTION

The Wiener number is defined as the half sum of distances between all pairs of vertices in a molecular graph, see: WIENER, 1947; GUTMAN and ŠOLTÉS, 1991; KLAVŽAR and ŽEROVNIK, 1996; DOBRYNIN *et al.*, 2001, 2002; VUKIČEVIĆ and GRAOVAC, 2004; KLAVŽAR and GUTMAN, 2006; WAGNER, 2006, 2010; ZHANG *et al.*, 2008, 2010; ZHOU and TRINAJSTIĆ, 2009; HEYDARI and GUTMAN, 2010; FURTULA, 2013; GHORBANI and GHORBANI, 2013; LIN, (2013a,b, 2014; GUTMAN and ŠKREKOVSKI, 2014; KOOREPAZAN-MOFTAKHAR and ASHRAFI, 2015; SHABANI and ASHRAFI, 2016.

Let G be a group and Ω be a non-empty set. An action of G on Ω is a function $\varphi: G \times \Omega \to \Omega$ where $(g,x) \mapsto \varphi(g,x)$ that satisfies the following two properties (we denote $\varphi(g,x)$ as x^g): $\alpha^e = \alpha$ for all α in Ω and $(\alpha^g)^h = \alpha^{gh}$ for all g,h in G. The orbit of an element $\alpha \in \Omega$ is denoted by α^G and it is defined as the set of all α^g, $g \in G$. The stabilizer of element $\alpha \in \Omega$ is defined as $G_\alpha = \{g \in G : \alpha^g = \alpha\}$. Let $H = G_\alpha$. Then for $\alpha, \beta \in \Omega$ $(\alpha \neq \beta)$, H_α is denoted by $G_{\alpha,\beta}$. On the other hand, the orbit-stabilizer theorem implies that $|\alpha^G|.|G_\alpha| = |G|$.

A bijection f on the vertices of graph X is called an automorphism of X which preserves the edge set E. In other words, the bijection f on $V(X)$ is an automorphism if $e=uv$ is an edge, then $f(e) = f(u)f(v)$ is an edge of E in which the image of vertex u is denoted by $f(u)$. The set of all automorphisms of X s denoted by $\mathrm{Aut(X)}$. It is not difficult to see that $\mathrm{Aut}(X)$ under the composition of mappings forms a group. This group acts transitively on the set of vertices, if for a pair of vertices such as u and v in $V(X)$, there is an automorphism $g \in \mathrm{Aut(X)}$ such that $g(u) = v$.

The modified Wiener index was introduced in 1991 by A. GRAOVAC and T. PISANSKI to count the symmetries of a graph, see [17]. The modified Wiener index is also called Graovac-Pisanski index as suggested M. GHORBANi and S. KLAVŽAR in [16]. Consider the graph X with automorphism group $G = \mathrm{Aut(X)}$. Then the Graovac-Pisanski index of X is

$$\hat{W}(\mathrm{X}) = \frac{|V(X)|}{2|G|}\sum_{u\in V(X)}\sum_{f\in G} d(u, f(u)) \qquad (1)$$

Theorem 1 (GRAOVAC and PISANSKI, 1991). Let X be a graph with automorphism group $G = \mathrm{Aut}(X)$ and vertex set V(X). Let V_1, V_2, …,V_k be all orbits under the action G on V(X). Then

$$\hat{\mathrm{W}}(X) = |\mathrm{V}(X)|\sum_{\mathrm{i}=1}^{\mathrm{k}}\frac{\mathrm{W}(\mathrm{V}_i)}{|\mathrm{V}_i|}. \qquad (2)$$

The difference between Wiener and modified Wiener indices is defined in HAKIMI-NEZHAAD and GHORBANI (2014) as

$$\delta(X) = \mathrm{W}(X) - \hat{\mathrm{W}}(X). \qquad (3)$$

It is clear that X is vertex-transitive if and only if the difference number is zero. Many properties of this topological index are studied in: KLEIN *et al.*, 1995; LIN, 2014; ASHRAFI *et al.*, 2015; ASHRAFI and DIUDEA, 2016; ASHRAFI and SHABANI, 2016; GHORBANI *et al.,* 2016; GHORBANI and HAKIMI-NEZHAAD, 2016, 2017; GHORBANI and KLAVŽAR, 2016. It can be resulted from Eq. (2) that the difference number is closely related to the number of orbits of Aut(X). In other words, the difference number is equal with the Wiener number if the regarded graph is asymmetric (a graph without non-trivial symmetry element). It is not difficult to see that in this case the number of orbits is equal with the number of vertices.

MAIN RESULTS AND DISCUSSION

A polyhedral graph is a 3-connected simple planar graph. GHORBANI *et al.* in a series of papers [ASHRAFI and GHORBANI, 2009, 2010; ASHRAFI *et al.*, 2010; GHORBANI, 2010, 2013; GHORBANI and GHORBANI, 2013; GHORBANI *et al.*, 2016; GHORBANI and HAKIMI-NEZHAAD, 2016, 2017] introduced some new classes of polyhedral graphs with tetragons, pentagons, heptagons and octagons. In this paper, we also introduce an infinite class of cubic polyhedral graphs with tetragons, pentagons and hexagons denoted by (4,5,6)-polyhedral graphs. This class of polyhedral graphs has exactly $16n$+8 vertices, where n is an integer greater than or equal with 3and thus, we denote this new family of cubic polyhedral graphs by C_{16n+8}, see Figures 1 and 2.

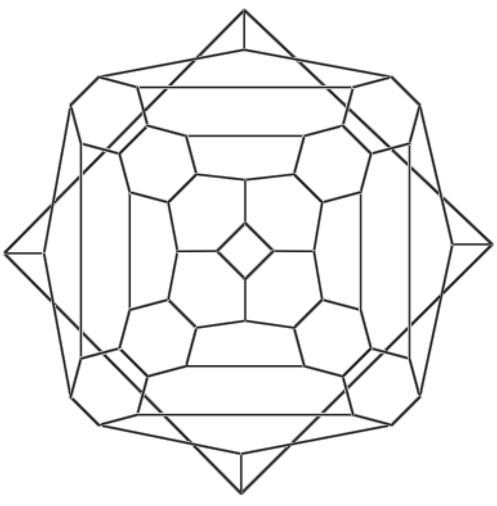

Figure 1. C_{16n+8} for n = 3.

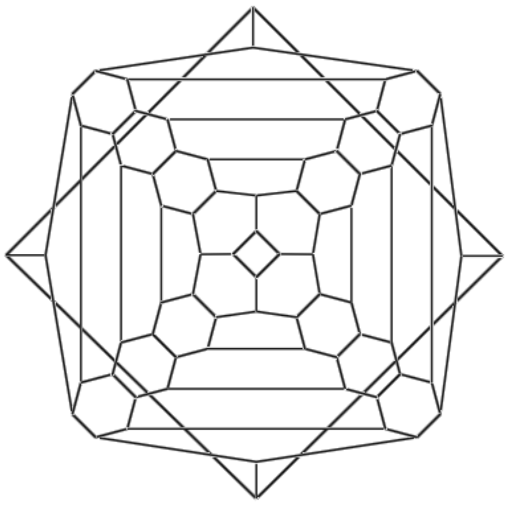

Figure 2. C_{16n+8} for n = 4.

Let s, p, h, n and m be respectively the number of tetragons, pentagons, hexagons, carbon atoms and bonds between them, in a given (4,5,6) polyhedral graph. By Euler's formula,we have

$$n - m+(s+p+h) = 2. \qquad (4)$$

Since this graph is cubic, we have

$$2m = 3n. \qquad (5)$$

On the other hand

$$4s + 5p + 6h = 2m. \qquad (6)$$

This yields $s = 2$, $p= 8$ and $h = 8n - 4$, for $n \geq 3$. Consider now the dihedral group D_{2n} with the following presentation:

$$D_{2n} = \left\langle a,\ b : a^n = b^2 = 1, b^{-1}ab = a^{-1} \right\rangle.$$

This group is considered as the symmetry group of many molecular graphs such as fullerenes and polyhedral graphs. This group is of order $2n$ with two generators of orders n and 2. The cyclic group $\mathbb{Z}_n$ of order n is also a group with generator g in which $\mathbb{Z}_n = \{g, g^2, ..., g^n = 1\}$.

Lemma 2. Let $n = 3$. The automorphism group of the graph C_{16n+8} is isomorphic with the group $\mathbb{Z}_2 \times D_8$.

Proof. The polyhedral graph C_{16n+8}, for n=3is depicted in Figure 3. Let G=Aut(C_{16n+8}). If α denotes the rotation of C_{16n+8} for 90° and β,γ are two reflections over the central vertical lines, then $G \geq \prec \alpha,\beta,\gamma \succ$. On the other hand, $|\prec \alpha,\beta,\gamma \succ| = 16$, where

$$\alpha^4 = \beta^2 = \gamma^2 = 1,\ \beta\alpha\beta=\alpha^{-1},\ \beta\gamma=\gamma\beta, \alpha\gamma=\gamma\alpha. \qquad (7)$$

Hence, one can verify that $\langle \alpha,\beta,\gamma \rangle \cong \mathbb{Z}_2 \times D_8$. On the other hand, the orbit-stabilizer theorem implies that $|G| = |1^G| \times |G_1|$. Next, consider the action of subgroup G_1. Any symmetry of the polyhedral graph C_{56} which fixes vertex 1 must also fixes the opposite vertex 3. Then applying again orbit-stabilizer property states that $|G_1| = |3^{G_1}| \times |G_{1,3}|$. It is not difficult to prove that $|G_{1,3}| = 2$ and $|3^{G_1}| = 1$. Hence, $|G_1| = 2$. On the other hand $1^G = \{1, 2, 3, 4, 53, 54, 55, 56\}$ and thus $|G| = 16$. This means that $G \cong \mathbb{Z}_2 \times D_8$.

Theorem 3. The automorphism group of the graph C_{16n+8} is isomorphic with the group $\mathbb{Z}_2 \times D_8$.

Proof. Similar to the proof of Lemma 2, suppose that α denotes the rotation of C_{16n+8} for 90° and that β,γ are two reflections over the central vertical lines. Then $G \cong \langle \alpha,\beta,\gamma \rangle \cong \mathbb{Z}_2 \times D_8$.

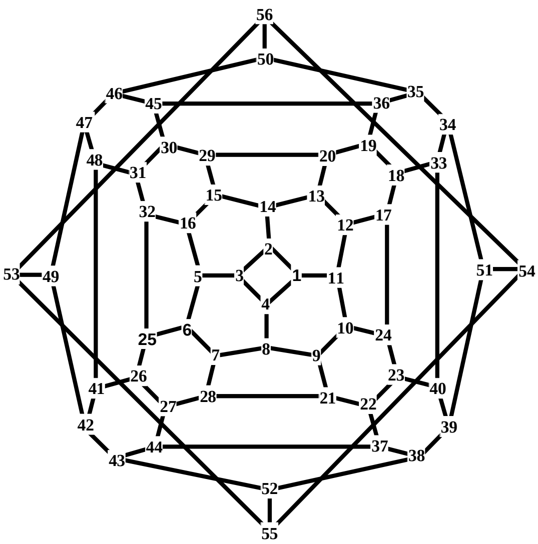

Figure 3. Labeling of the polyhedral graph C_{16n+8} for n=3.

Theorem 4. Consider the nanotube L depicted in Figure 4. For $n \geq 3$

$$W(L)=\frac{256}{3}n^3+128n^2+\frac{320}{3}n-224, \tag{8}$$

where n + 1 is the number of layers of L.

Proof. Suppose the vertices of the last layer are $U = \{u_1, u_2, \ldots, u_{16}\}$. Let t_n be two times the Wiener index of graph L. A straightforward computation yields the recurrence

$$\begin{aligned}2W(L)=t_n &= \sum_{x,y\in U} d(x,y)+\sum_{x,y\in V\setminus U} d(x,y)+2\sum_{x\in U,y\in V\setminus U} d(x,y)\\ &=1024+t_{n-1}+2\sum_{x\in U,y\in V\setminus U} d(x,y).\end{aligned} \tag{9}$$

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

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

Where $d(u_1)=\sum_{y\in V\setminus U} d(u_1,y)$ and $d(u_2)$ is defined similarly, see Figure 4. By computing these values, one can see that:

$$\begin{aligned}d(u_1)&=16n^2-8n-12,\\ d(u_2)&=16n^2+8n-44.\end{aligned} \tag{10}$$

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

$$W(L)=\frac{256}{3}n^3+128n^2+\frac{320}{3}n-224. \tag{11}$$

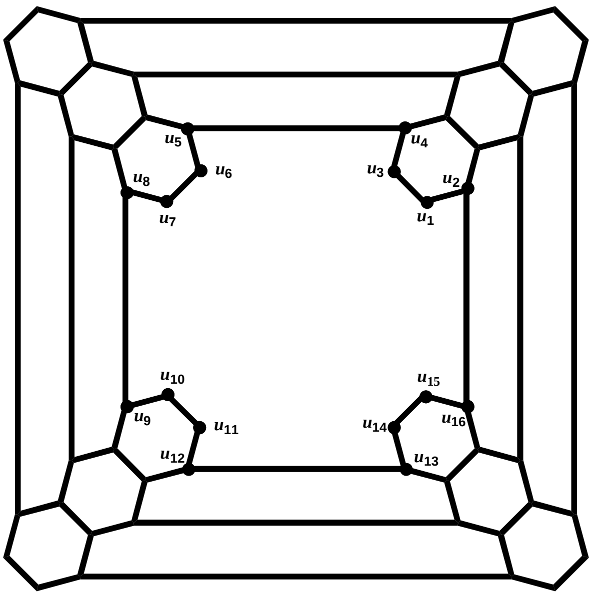

Figure 4. 2 - D graph of nanotube L.

Theorem 5. For $n \geq 3$, we have

$$W(C_{16n+8})=\frac{256}{3}n^3+384n^2+\frac{1664}{3}n-324. \tag{12}$$

Proof. First we partite the vertices of graph into three subsets B, U and W, where $B = \{v_1, v_2, \ldots, v_r\}$, $U = \{u_1, \ldots, u_s\}$ and $W = \{w_1, \ldots, w_r\}$ are respectively the set of vertices of the internal cap, the vertices of nanotube L and the vertices of outer cap, see Figure 5. The distance matrix D can be written as following block form:

$$D = \begin{pmatrix} V & B & W \\ B & U & B \\ W & B & V \end{pmatrix}.$$

The entries of matrix U is computed in Theorem 4. 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 given polyhedral graph C_{16n+8}, the matrix V is constant as shown in Figure 6. The summation of entries of matrix V is 696. Obviously, the distance matrices B, U, and W depend to the number of rows in the nanotube L.

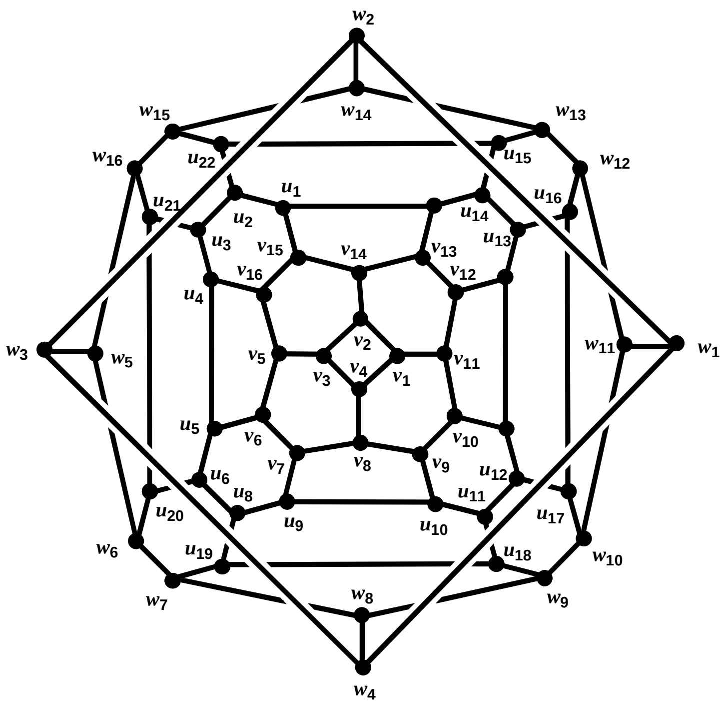

Figure 5. Labeling of the polyhedral graph C_{16n+8} for n=3.

In other words, if w_n and $w_{n\text{-}1}$ are the Wiener indices of the polyhedral graphs C_{16n+8} and $C_{16(n-1)+8}$, respectively, then similar to the proof of the Theorem 1, for $n \geq 4$, we have:

$$w_4 - w_3 = 6400, w_5 - w_4 = 9216, w_6 - w_5 = 12544, w_7 - w_6 = 16384. \quad (13)$$

Again, a straightforward computation yields the recurrence

$$w_n - w_{n-1} = 256n^2 + 512n + 256. \qquad (14)$$

The solution of this recurrence is

$$\mathrm{W}(\mathrm{C}_{16n+8}) = \frac{256}{3}n^3 + 384n^2 + \frac{1664}{3}n - 324. \qquad (15)$$

This completes the proof.

Corollary 6. For the polyhedral graph C_{16n+8}, we have

$$\delta(C_{16n+8}) = \frac{64}{3}n^3 - 96n^2 + \frac{776}{3}n - 360 \quad n \geq 3. \tag{16}$$

Proof. By using Theorem 3, for $n \geq 3$, we have $\mathrm{Aut}(C_{16n+8}) \cong \mathbf{Z}_2 \times D_8$. By using Eq. (2), similar to the proof of Theorem 4, one can conclude that

$$\hat{\mathrm{W}}(C_{16n+8}) = 64n^3 + 480n^2 + 296n + 36. \tag{17}$$

This completes the proof.

CONCLUSION

In this paper, we introduced a new family of cubic polyhedral graphs and then we computed its Graovac-Pisanski index. We also computed the difference between Wiener and *GP* indices for this class of polyhedral graphs.

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

Figure 6.

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