Differences between Wiener and modified Wiener indices

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ABSTRACT. The Wiener index is the oldest topological index introduced by H. Wiener for anticipating the boiling point of Paraffin and some other alkenes. An algebraic approach for generalizing the Wiener index is proposed by Graovac and Pisanski for the first time. In this paper, we compute the difference between these topological indices for a class of fullerene graphs.

Keywords: Wiener index, molecular graph, automorphism of graph.

1. INTRODUCTION

A graph is a collection of points and lines connecting them. We call these points and lines by vertices and edges and we denote them by $V(\Gamma)$ and $E(\Gamma)$, respectively. Two vertices x and y are adjacent if $xy \in E(\Gamma)$.

The distance between any pair of vertices $x, y \in V(\Gamma)$ is defined as the length of the shortest path between them denoted by $d(x,y)$. A connected graph is one whose all pairs of vertices are connected by a path. A simple graph is a graph without loop and parallel edges. A molecular graph or a chemical graph is a labeled simple graph whose

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vertices and edges correspond to the atoms and chemical bonds, respectively. In a molecular graph, it is convenient to omit hydrogen atoms.

Let Ω be the class of all connected graphs, a topological index for a graph Γ is a function $f : \Omega \to \mathbb{R}^+$ which is invariant under its automorphisms. The Wiener index is the first reported distance based topological index and is defined as half sum of the distances between all the pairs of vertices in a molecular graph, see [14,18]. We can consider the Wiener index as a function $W: \Omega \to \mathbb{Z}^+$ which is not onto. For example there is no graph such as G with $W(G) = 2$. Milan Randić in 1993 defined the hyper–Wiener index of acyclic graphs and then Klein et al. [15] generalized Randić's definition for all connected graphs, as a generalization of the Wiener index. It is defined as

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

We refer to [11-13] for mathematical properties and chemical meaning of this topological index.

2. RESULTS AND DISCUSSIONS

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

Graovac and Pisanski [10] proposed an algebraic approach for generalizing the Wiener index by automorphism group of the graph under consideration. Assume that Γ is a graph with automorphism group G = Aut(Γ), then the modified Wiener index of Γ is defined as:

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

They introduced this generalization of the classical Wiener index to consider into account the symmetry structure of the graph Γ. Koorehpazan-Moftakhar et al. in [16] defined the modified hyper–Wiener index of Γ as follows:

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

Theorem 1 [10]. Let Γ is a graph with automorphism group G = Aut(Γ) and vertex set $V(\Gamma)$. Let $V_1, V_2, ..., V_k$ be all orbits of action G on $V(\Gamma)$. Then

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

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

Throughout this paper we use standard notations of graph theory. It is easy to see that the Wiener index is equal with modified Wiener index if and only if Γ is vertex-transitive and the modified Wiener index is zero if and only if Aut(Γ) is trivial. For given graph Γ the difference between Wiener and modified Wiener indices can be defined as follows:

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

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

$$\delta\delta(\Gamma) = WW(\Gamma) - \overset{\wedge}{WW}(\Gamma).$$

Example 1. It is easy to see that the symmetry group of complete graph K_n is isomorphic to the symmetric group S_n and so K_n is vertex-transitive. Thus Corollary 2 implies that $\delta(\Gamma) = 0$.

Example 2. Let $ST(n)$ is a star on n vertices, then the vertices of $ST(n)$ can be divided into sets: the vertex of degree $n-1$ compose an orbit and the other vertices compose the second orbit. On the other hand, $Aut(ST(n)) \cong S_{n-1}$ and hence,

$$W\big(ST(n)\big) = \frac{1}{2}\sum_{u\in V}\sum_{v\in V}d(u,v) = \big(n-1\big)^2,$$
$$\hat{W}(ST(n)) = \frac{|V(S_n)|}{2\,|\,Aut(S_n)|}\sum_{\alpha\in Aut(S_n)}\sum_{v\in V}d(v,\alpha(v))$$
$$= (n-1)\times\frac{n}{2(n-1)!}\times 2\times(n-2)(n-2)! = n(n-2).$$

This leads us to conclude that $\delta(ST(n)) = (n-1)^2 - n(n-1) = 1$.

A fullerene is a molecule composed of carbon atoms in the form of many shapes such as hollow sphere, ellipsoid, tube, etc. The most important fullerenes are spherical fullerenes or buckyballs. Carbon nanotubes or buckytubes are cylindrical fullerenes, [6,17]. Fullerenes are similar in structure to graphite, but they may also contain triangle, square, pentagonal, hexagonal or sometimes heptagonal rings, [7]. The molecular graph of a given fullerene molecule is called a fullerene graph.

Theorem 3 (Euler's Formula). Let Γ be a planar graph and n, m, f are the number of vertices, edges and faces, respectively. Then

$$n - m + f = 2.$$

Behmaram [1] extended the definition of fullerene to m-generalized fullerene. By his definition, a 3-connected cubic planar graph Γ is called m-generalized fullerene

if its faces are two *m*-gons and all other pentagons and hexagons. For other generalization of fullerenes, see Refs [2-5]. In the mentioned papers several deep results by Deza and his co-authors about these molecular graphs were introduced. Following their method Ghorbani in [7] introduced a new class of fullerene with pentagons and heptagons. In this paper, we also introduce an infinite class of fullerene with squares, pentagons and hexagons, see Figure 1. This class of fullerenes has exactly 16*n* + 4 vertices where *n* is an integer greater than or equal with 2. That's why we name this new family of fullerene graphs by C_{16n+4}. Let s, *p, h, n* and *m* be the number of squares, pentagons, hexagons, carbon atoms and bonds between them, in a given (4,5,6) fullerene *F*. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is *n* = (4s + 5*p* + 6*h*)/3, the number of edges is *m* = (4*s* + 5*p* + 6*h*)/2 = 3/2*n* and the number of faces is *f* = s+ *p* + *h*. By the Euler's formula *n* − *m* + *f* = 2, one can deduce that s + *p* + *h* = 2 + *n*/2. This leads up to conclude that *s*=3 and *p*= 6 and *h* = 8*n-5,* for *n* ≥ 2. Two members of this class of fullerenes are depicted in Figures 2, 3.

Theorem 4. Aut$(C_{16n+4}) \cong \mathbb{Z}_2 \times \mathbb{Z}_2$.

Proof. We calculate the order of the group G = Aut(C_{16n+4}) of symmetries of the fullerene C$_{16n+4}$, for *n*=2 depicted in Figure 1 and the automorphism group of C_{16n+4} in general can be computed similarly. Suppose α is a reflection as follows:
α=(1,4) (2,3) (5,6) (7,20) (8,19)(9,18)(10,17)(11,16)(12,15)(13,14)(21,26) (22,25) (23,24)(27,32)(28,31)(29,30)(33,34)(35,36).

Thus the orbit of the subgroup <α> is $1^{<\alpha>}$ ={1,4}. Now, consider the axis symmetry element which fixes vertices {1,4,10,17}, it is as follows:
β=(2,6)(3,5)(7,13)(8,12)(9,11)(14,20)(15,19)(16,18)(21,32)(22,31)(23,30)(24,29) (25,28)(26,27)(33,36)(34,35).

Clearly, $G \geq \prec \alpha, \beta \succ$. Now the orbit-stabilizer property shows that $|G| = |1^G| \times |G_1|$. Next consider the action of subgroup G_1. Any symmetry of the fullerene C$_{16n+4}$ which fixes vertex 1 must also fix the opposite vertex 4. Then applying again orbit-stabilizer property states that $|G_1| = |4^{G_1}| \times |G_{14}|$. It is easy to prove that $|G_{14}|$ = 1, $|4^{G_1}| = 2$ and hence $|G|$ = 4. On the other hand, $|\prec \alpha, \beta \succ| = 4$ where $\alpha^2 = \beta^2 = 1, \beta\alpha = \alpha\beta$. This leads us to conclude that Aut$(C_{16n+4}) \cong \mathbb{Z}_2 \times \mathbb{Z}_2$.

Corollary 5. For the fullerene graph C_{16n+4} for *n* ≥ 3, we have

$$\delta(C_{16n+4}) = \frac{256}{3}n^3 - 192n^2 + \frac{1808}{3}n - 390,$$
$$\delta\delta(C_{16n+4}) = \frac{128}{3}n^4 + 256n^3 - \frac{4046}{3}n^2 + 3504n - 2375.$$

Proof. At first by a direct computation, we have $W(C_{36}) = 2330$ and $WW(C_{36}) = 6221$. By applying the methods of [8,9] one can see that for *n* ≥ 3:

$$W(C_{16n+4}) = \frac{256}{3}n^3 + 320n^2 + \frac{1184}{3}n - 474,$$
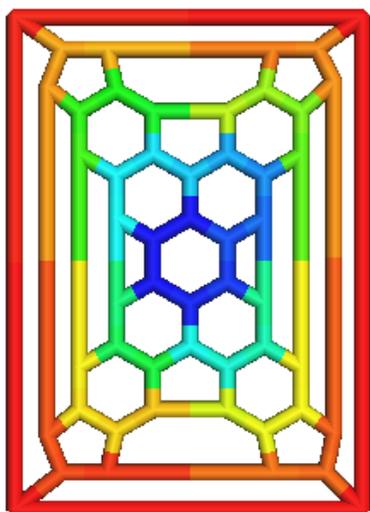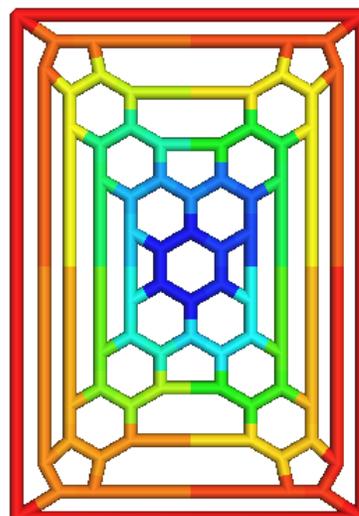$$WW(C_{16n+4}) = \frac{128}{3}n^4 + 256n^3 + \frac{1792}{3}n^2 + 1824n - 2917. \qquad (1)$$
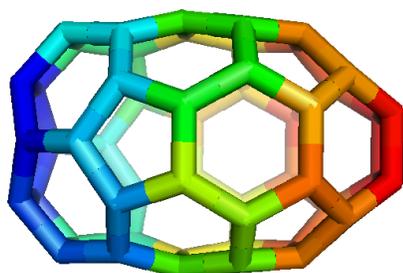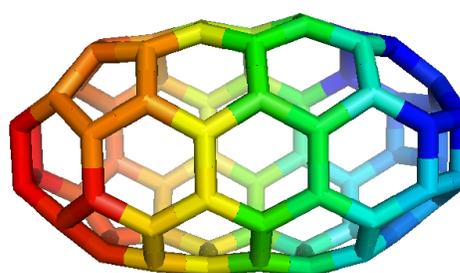
On the other hand, by using Theorem 4, $\hat{W}(C_{36}) = 1620$, $\hat{WW}(C_{36}) = 4464$ and for $n \geq 3$ we have:

$$\hat{W}(C_{16n+4}) = 512n^2 - 208n - 84,$$
$$\hat{WW}(C_{16n+4}) = 1952n^2 - 1680n - 542. \qquad (2)$$

The proof can be resulted from *Eq.* (1) and *Eq.* (2).
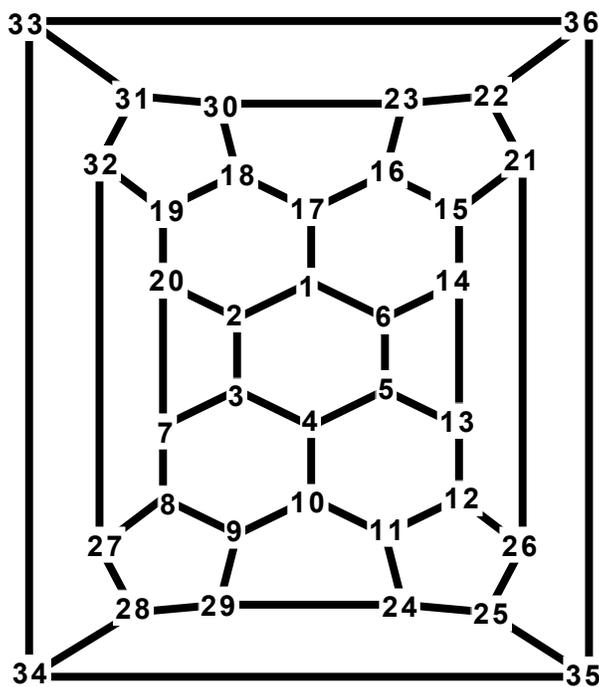
Figure 1. Labeling of fullerene C_{16n+4} for *n*=2.

2-*D* graph of C_{16n+4} for $n = 3$.

2-*D* graph of C_{16n+4} for $n = 4$.

Figure 2. The Case of $n = 3$ in C_{16n+4}.

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

3.   CONCLUSION

In this paper, we studied some properties of the modified Wiener and modified hyper-Wiener indices. We also introduced a new family of fullerene graphs and then we computed these new topological indices for them. Finally, we proposed two new topological indices regarding to the modified Wiener indices groups and we studied some properties of them.

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