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WIENER AND HYPER WIENER INDEX OF GRAPHS

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***Abstract*:** The Wiener index is one of the oldest graph parameter which is used to study molecular-graph-based structure. This parameter was first proposed by Harold Wiener in 1947 to determining the boiling point of paraffin. The Wiener index of a molecular graph measures the compactness of the underlying molecule. This parameter is wide studied area for molecular chemistry. It is used to study the physio-chemical properties of the underlying organic compounds. The Wiener index of a connected graph is denoted by

$$W(G) = \frac{1}{2}\sum_{u,v\in V_G} d_G(u,v),$$

that is $W(G)$ is the sum of distances between all pairs (ordered) of vertices of G .In this paper we will find the Hyper Wiener index which is defined as ,

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{4}\sum_{u,v\in V_G} d_G^2(u,v), \ where \ d_G^2(u,v) = d_G(u,v)^2$$

***Keywords*:** Wiener index, Hyper Wiener index, Molecular graph.

INTRODUCTION

All graphs considered in this paper are simple and connected. One of the oldest and well-studied distance based graph invariants associated with a connected graph G is the *Wiener number* $W(G)$, also termed as *Wiener index* in chemical or mathematical chemistry literature, which is defined [8] as the sum of distance over all unordered vertex pairs in G, namely,

$$W(G) = \sum_{u,v\in V_G} d_G(u,v).$$

For more results on wiener index one may be referred to those in Dobrynin and Kochetova [9] and its references. Dobrynin and Kochetova [9] and Gutman [12] independently proposed a vertex degree-weighted version of the Wiener index called the degree distance or the Schultz molecular topological index, which is defined for a connected graph G as

$$DD(G) = \frac{1}{2}\sum_{u,v\in V_G} (d_G(u)+d_G(v))d_G(u)d_G(v)$$

where $d_G(u)$ is the degree of the vertex u in G. Note that the degree distance is a degree-weight version of the Wiener index. Many results on the degree distance DD(G) have been put forward in past decades, and they mainly deal with extreme properties of $DD(G)$. Tomescu [4] showed that the star is the unique graph with minimum degree distance within the class on n-vertex connected graphs. Tomescu [4] deduced properties of graphs with minimum degree distance in the class of n-vertex connected graphs with $m \geq n-1$ edges.

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The hyper-Wiener index of acyclic graphs was introduced by Milan Randic in 1993. Then Klein et al. [6], generalized Randics definition for all connected graphs, as a generalization of the Wiener index. It is defined as

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{4}\sum_{u,v\in V_G} d_G^2(u,v), \ where \ d_G^2(u,v) = d_G(u,v)^2$$

We encourage the reader to consult [10]-[16] for the mathematical properties of hyper-Wiener index and its applications in chemistry.

For example in the Fig. 1, gives the picture of a molecule structure of benzyl and the corresponding molecular graph.

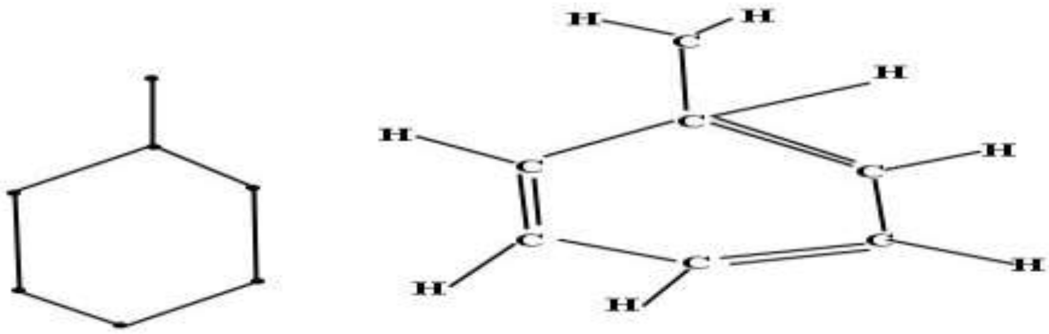

Fig. 1

Theorem 1.1. Let G be a connected graph with size n and m .Then

$$WW(G) = \frac{3n^3}{4} - n^2 + \frac{n}{4} - m$$

Proof. Suppose G be a graph of order n and size m with diameter $(G) \le 2$. Define the sets $A = u \in V \mid e(u) = 1$ and $B = u \in V \mid e(u) = 2.$ Then, $|A| + |B| = n.$ If $u \in A,$ then $d_G(u,v) = n-1$ and if $u \in B,$ then define two sets B_1 and B_2 as $B_1 = v \in V \mid d(u,v) = 1$ and $B_2 = v \in V \mid d(u,v) = 2$.

Then

$$d_G(u,v) = |B_1| + 2|B_2| = |B_1| + |B_2| + |B_2|$$

since $|B_1| + |B_2| = n-1,$

thus

$$\begin{aligned} d_G(u,v) &= n-1+(n-1-|B_1|) \\ &= 2n-2-|B_1| \\ &= 2n-2-d_G(u). \end{aligned}$$

$$W(G) = \frac{1}{2}\sum_{u,v\in V_G} d_G(u,v).$$

$$= \frac{1}{2}\left\{\sum_{u\in A} d_G(u,v) + \frac{1}{2}\sum_{u\in B} d_G(u,v)\right\}$$

$$= \frac{1}{2}\{(n-1)|A| + (2n-2-d_G(u))|B|\}$$

$$= \frac{1}{2}\left\{(n-1)|A| + (2n-2)|B| - \sum_{u\in B} d_G(u)\right\}$$

$$= \frac{1}{2}\left\{(n-1)(|A|+|B|) + (n-1)|B| - \sum_{u\in B} d_G(u)\right\}$$

$$= \frac{1}{2}\left\{n(n-1) + (n-1)(n-|A|) - \sum_{u\in B} d_G(u)\right\}$$

$$= \frac{1}{2}\left\{n(n-1) + n(n-1) - (n-1)|A| - \sum_{u\in B} d_G(u)\right\}$$

Therefore, $$= \frac{1}{2}\left\{2n(n-1) - \sum_{u\in A} d_G(u) - \sum_{u\in B} d_G(u)\right\}$$

$$= \frac{1}{2}\left\{2n(n-1) - \sum_{u\in V} d_G(u)\right\} = \frac{1}{2}\{2n(n-1) - 2m\} \qquad Since \sum_{u\in V} d_{(}u) = 2m$$

$$= n^2 - n - m$$

Now for finding Hyper Wiener index we have;

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{4}\sum_{u,v\in V_G} d_G^2(u,v), \ where \ d_G^2(u,v) = d_G(u,v)^2$$

$$
\begin{aligned}
WW(G) = \quad & \frac{1}{2}(n^2-n-m)+\frac{1}{4}(\{(n-1)^2\,|A|+(3(n-1)^2-4(n-1)-d_G(u)d_G(u))\,|B|)\} \\
&= \frac{1}{2}(n^2-n-m)+\frac{1}{4}(\{(n-1)^2\,|A|+3\,|B|\,(n-1)^2-(4(n-1)-d_G^2(u))\,|B|)\} \\
&= \frac{1}{2}(n^2-n-m)+\frac{1}{4}(\{n(n-1)^2+2\,|B|\,(n-1)^2-(4(n-1)-d_G^2(u))\,|B|)\} \\
&= \frac{1}{2}(n^2-n-m)+\frac{1}{4}(\{n(n-1)^2+2(n-|A|)(n-1)^2-(4(n-1)-d_G(u))\,|B|)\} \\
&= \frac{1}{2}(n^2-n-m)+\frac{1}{4}(\{n(n-1)^2+2n(n-1)^2-2(n-1)^2\,|A|-(4(n-1)-d_G^2(u))\,|B|)\} \\
&= \frac{1}{2}(n^2-n-m)+\frac{1}{4}(\left\{3n(n-1)^2-\sum_{u\in A}d_G(u)-\sum_{u\in B}d_G(u))\right\} \\
&= \frac{1}{2}(n^2-n-m)+\frac{1}{4}(3n(n-1)^2-\sum_{u\in V}d_G(u)) \\
&= \frac{1}{2}(n^2-n-m)+\frac{1}{4}[3n(n-1)^2-2m] \\
&= \frac{n^2}{2}-\frac{n}{2}-\frac{m}{2}+\frac{3}{4}(n(n^2+1-2n)-2m) \\
&= -n^2+\frac{3n^3}{4}+\frac{n}{4}-m \\
&= \frac{3n^3}{4}-n^2+\frac{n}{4}-m
\end{aligned}
$$

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