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The multiply version of Zagreb indices of a family of molecular graph "polycyclic aromatic hydrocarbons (PAHS)"

Mohammad Reza Farahani[1] and Wei Gao[2]

[1]*Department of Applied Mathematics of Iran University of Science and Technology (IUST), Narmak, Tehran, Iran*
[2]*School of Information Science and Technology, Yunnan Normal University, Kunming, China*

ABSTRACT

Let G is an arbitrary simple, connected, graph, with the vertex set V(G) and edge set E(G). In chemical graph theory, we have many invariant polynomials and topological indices for a molecular graph, with applied in chemical and nano science and vice versa. Topological indices are numerical parameters of a molecular graph G which characterize its topology. The First Zagreb index $Zg_1(G)=\sum_{uv\in E(G)}(d_u+d_v)$, *Second Zagreb index* $Zg_2(G)=\sum_{uv\in E(G)}(d_u\times d_v)$ *are the oldest graph invariants used in mathematical chemistry to predict the chemical phenomena. In this paper, we compute the multiply vetsion of Zagreb indices of a family of molecular graph "Polycyclic Aromatic Hydrocarbons (PAHs)".*

Keywords: Molecular graphs, Polycyclic Aromatic Hydrocarbons, Zagreb indices, Multiple Zagreb indices.

INTRODUCTION

Let $G=(V,E)$ be a simple graph with $n=|V=V(G)|$ vertices and $e=|E=E(G)|$ edges. In chemical graph theory, then its vertices correspond to the atoms and the edges to the bonds. Throughout this paper, we denoted The vertex set, edge set, the number of vertices, edges and the degree of a vertex v (The degree d_v of a vertex $v\in V(G)$ is the number of vertices of G adjacent to v.) of a molecular graph G by $V(G)$, $E(G)$, υ, e and d_v, respectively . And $\forall u,v\in V$, the distance $d(u,v)$ is defined as the length of the shortest path between u and v in G. A general reference for the notation in graph theory is [1-4].

Topological indices are numerical parameters of a molecular graph G which characterize its topology. There exits many structure in graph theory, with applied in chemical and nano science and vice versa and computing the connectivity indices of molecular graphs is an important branch in chemical graph theory.

An important and oldest topological index introduced more than forty years ago by *I. Gutman* and *N. Trinajstić* is the *First Zagreb index* $M_1(G)$ [5]. It is defined as the sum of squares of the vertex degrees d_u and d_v of vertices u and v in G. Recently, we know *Second Zagreb index* $Zg_2(G)$, and the first and second Zagreb indices are defined as:

$$M_1(G)=\sum_{e=uv\in E(G)}(d_v+d_v) \text{ or } M_1(G)=\sum_{v\in V(G)} d_v^2$$

$$M_2(G)=\sum_{e=uv\in E(G)}(d_v\times d_v)$$

In 2012, *M. Ghorbani* and his co-authors [6] introduced two new versions of Zagreb indices of a graph *G*, based on degree of vertices of *G*. The *Multiple Zagreb* topological indices are defined as [7-16]:

$$PM_1(G)=\prod_{e=uv\in E(G)}(d_v+d_v)$$

$$PM_2(G)=\prod_{e=uv\in E(G)}(d_v\times d_v)$$

Some basic properties of $M_1(G)$ can be found in some recent papers [17-28].

The aim of this paper is to compute the multiply vetsion of first and second Zagreb indices of a family of molecular graph "*Polycyclic Aromatic Hydrocarbons (PAH)*".

RESULTS AND DISCUSSION

In this section, we focus on the structure of hydrocarbon structures and counting the First Multiple Zagreb index and Second Multiple Zagreb index of *Polycyclic Aromatic Hydrocarbons PAH.* The *Polycyclic Aromatic Hydrocarbons PAHn* is a family of hydrocarbon molecules, such that its structure is consisting of cycles with length six (Benzene).

Polycyclic Aromatic Hydrocarbons can be thought as small pieces of graphene sheets with the free valences of the dangling bonds saturated by *H. Vice versa*, a graphene sheet can be interpreted as an infinite PAH molecule. Successful utilization of PAH molecules in modeling graphite surfaces has been reported earlier [28-46] and references therein.

In this paper, we denote and shown two famous first members of this hydrocarbon family as follows:
PAH_1 be the *Benzene* with six carbon (C) and six hydrogen (H) atoms.
PAH_2 be the *Coronene* with 24 carbon and twelve hydrogen atoms.

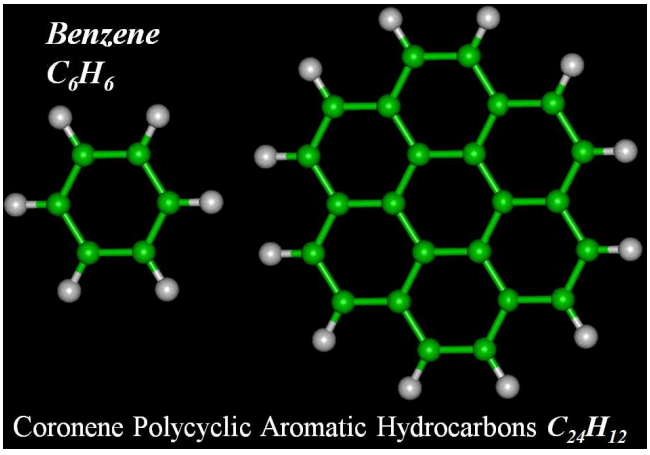

Figure 1. The first three graphs of *Polycyclic Aromatic Hydrocarbons* PAH_n

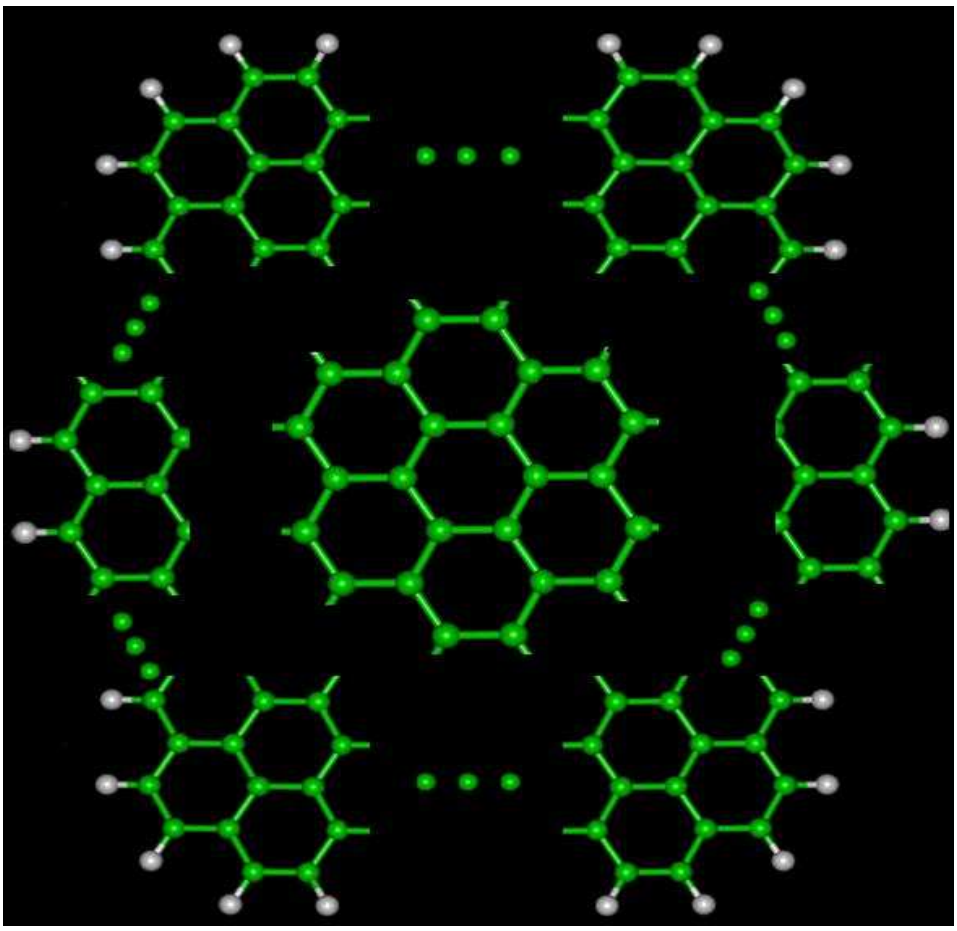

Figure 2. A general case of the Polycyclic Aromatic Hydrocarbons PAH_k with vertices/atoms and edges/bonds coloring

Theorem 1. [28] Let PAH_k be the k^{th} growth of Polycyclic Aromatic Hydrocarbons $\forall k \geq 1$. Then:

The First Zagreb index of PAH_k is equal to

$$M_1(PAH_k) = 54k^2+6k$$

The Second Zagreb index of PAH_k is equal to

$$M_2(PAH_k) = 81k^2-3k.$$

Theorem 2. Let PAH_k be the k^{th} growth of Polycyclic Aromatic Hydrocarbons $\forall k \geq 1$. Then:

The First Multiple Zagreb index of PAH_k is equal to

$$PM_1(PAH_k)=(2)^{(9k2+9k)}\times(3)^{(9k2-3k)}$$

The Second Multiple Zagreb index of PAH_k is equal to

$$PM_2(PAH_k)=(3)^{18k2}$$

Proof. Consider the k^{th} growth of Polycyclic Aromatic Hydrocarbons PAH_k, $k \geq 1$. In general case of this hydrocarbon molecular graphs, there are $6k^2+6k$ vertices/atoms ($=|V(PAH_k)|$).

From the general structure of PAH_k, one can see $6k^2$ of them are Carbon atoms and also $6k$ of them Hydrogen atoms, such that all Carbon atoms have degree 3 and Hydrogen atoms have degree one. In other words, we have two partitions of the vertex set $V(PAH_k)$ as follow

$$H=V_1=\{v\in V(PAH_k)|d_v=d_H=1\} \rightarrow |V_1|=6k$$
$$C=V_3=\{v\in V(PAH_k)|d_v=d_C=3\} \rightarrow |V_3|=6k^2$$

Thus, the number of edges/chemical-bonds in this hydrocarbon molecule is equal to:

$$|E(PAH_k)|=½[1\times 6k+3\times 6k^2]=9k^2+3k$$

Now, we have two partitions of the edge set PAH_k as follow

$$E_4=E_3^*=\{e=uv\in E(PAH_k)|\ d_u=d_H=1\ \&\ d_v=d_C=3\} \rightarrow |E_4|=6k$$
$$E_6=E_9^*=\{e=uv\in E(PAH_k)|\ d_u=d_v=d_C=3\} \rightarrow |E_6|=9k^2-3k$$

We mark the edges of E_4 or E_3) by gray color and the edges of E_6 or E_9^* by green color in Figure 1 and Figure 2, then the first and second Multiple Zagreb indices of the k^{th} growth of Polycyclic Aromatic Hydrocarbons PAH_k are equal to

$$PM_1(PAH_k)=\prod_{uv\in E(PAH_k)}\left(d_v+d_v\right)$$
$$=\prod_{uv\in E_4}\left(d_v+d_v\right)+\prod_{uv\in E_6}\left(d_v+d_v\right)$$
$$=(4)^{6k}\times(6)^{(9k2-3k)}$$
$$=(2)^{(9k2+9k)}\times(3)^{(9k2-3k)}$$

And the second Multiple Zagreb index of H_k is equal to

$$PM_2(PAH_k)=\prod_{uv\in E(PAH_k)}\left(d_v\times d_v\right)$$
$$=\prod_{uv\in E_3^*}\left(d_v\times d_v\right)+\prod_{uv\in E_9^*}\left(d_v\times d_v\right)$$
$$=(3)^{6k}\times(9)^{(9k2-3k)}$$
$$=(3)^{18k2}$$

Here, we complete the proof of Theorem 2.

CONCLUSION

In this paper, we compute two new topological indices “the First Multiple Zagreb index and Second Multiple Zagreb index” of a family of hydrocarbon molecular graphs " Polycyclic Aromatic Hydrocarbons PAH_k ".

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