Zagreb Indices and Zagreb Polynomials of Polycyclic Aromatic Hydrocarbons PAHs

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1. Introduction

Let $G$ be a simple connected molecular graph in chemical graph theory, then its vertices correspond to the atoms and the edges to the bonds. Throughout this paper, we denote the vertex set, edge set, the number of vertices, edges and the degree of a vertex $v$ (the number of its joining vertices) of a molecular graph $G$ by $V(G)$, $E(G)$, $v$, $e$ and $d_v$, respectively [1, 2].

In chemical graph theory, the topological indices of a molecular graph $G$ are a number relation to the structure of $G$ and are invariant on the automorphism of the graph. Chemical graph theory is an important branch of graph theory, such that there exits many topological indices in it and computing topological indices of molecular graphs is an important branch of chemical graph theory.

An important topological index introduced more than forty years ago by I. Gutman and N. Trinajstic is the First Zagreb index $Zg_1(G)$ [3-4]. 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 $Zg_2(G)$ [5]. First Zagreb index $Zg_1(G)$ and Second Zagreb index $Zg_2(G)$ formulated as follow:

$$Zg_1(G) = \sum_{u,v \in E(G)} (d_u + d_v)$$

$$Zg_2(G) = \sum_{u,v \in E(G)} (d_u \times d_v)$$

Also, we know two polynomials of two above indices. These are First Zagreb polynomial $Zg_1(G,x)$ and Second Zagreb polynomial $Zg_2(G,x)$ and are equal as follow

$$Zg_1(G,x) = \sum_{u,v \in E(G)} x^{d_u + d_v}$$

$$Zg_2(G,x) = \sum_{u,v \in E(G)} x^{d_u \times d_v}$$

We can obtain First Zagreb index $Zg_1(G)$ and Second Zagreb index $Zg_2(G)$ from its polynomial, because for $i=1,2$

$$Z_{g_i}(G) \mid_{x=1} = \frac{\partial Z_{g_i}(G,x)}{\partial x} \mid_{x=1}$$

Some basic properties of $Zg_i(G)$ can be found in some recent papers [3-13]. The goal of this paper is computing the first Zagreb index, second Zagreb index, first Zagreb polynomial and second Zagreb polynomial of a family of hydrocarbon structures "Polycyclic Aromatic Hydrocarbons (PAHs)"

2. Main Results and discussion

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 [14-27] and references therein.

In this paper, we denote the first members of this hydrocarbon family as follow and are shown in Figure 1:

\[ PAH_1 \] be the Benzene with six carbon (C) and six hydrogen (H) atoms, \[ PAH_2 \] be the Coronene with 24 carbon and twelve hydrogen atoms, \[ PAH_3 \] be the Circumcoronene with 54 carbon and eighteen hydrogen atoms.

**Figure 1.** The first three graphs of polycyclic aromatic hydrocarbon \( PAH_n \)

It is easy to see that the general representation of polycyclic aromatic hydrocarbon \( PAH_n \) has \( 6n^2 \) carbon (C) atoms and \( 6n \) hydrogen (H) atoms.

This polycyclic aromatic hydrocarbons (or PAH family) are very similar properties to one of famous family of Benzenoid system (Circumcoronene Homologous Series of Benzenoid). The properties and applications of Benzenoid system are presented in many papers; reader can see references [28-52]. The properties and applications of Benzenoid system are presented in many papers; reader can see references [28-52].

Now, before counting our favorites topological indices and properties such as the number of them are carbon atoms and also \( 6n \) of them are hydrogen atoms. Thus, the number of edge in this hydrocarbon molecule (chemical bonds) is equal to:

\[
|E(PAH_n)| = \frac{3 \times 6n^2 + 1 \times 6n}{2} = 9n^2 + 3n
\]

Now, if we mark the edges of \( E_4 \) (or \( E_4^* \)) by blue color and the edges of \( E_6 \) (or \( E_6^* \)) by yellow color in Figure 2, then we have the number of \( |E_4| = 6n \) and \( |E_6| = 9n^2 - 3n \) members edges of edge sets \( E_4 \) (or \( E_4^* \)), and \( E_6 \) (or \( E_6^* \)) of polycyclic aromatic hydrocarbon \( PAH_n \), respectively.

By according to the definition of First Zagreb polynomial and Second Zagreb polynomial, thus

\[
Z_{g1}(PAH_n) = \sum_{e \in E(PAH_n)} x^{d_c + d_e} = \sum_{e \in E_4^*} x^{6} + \sum_{e \in E_6^*} x^{4} = (9n^2 - 3n)x^4 + (6n)x^6
\]

And

\[
Z_{g2}(PAH_n) = \sum_{e \in E(PAH_n)} x^{d_c + d_e} = \sum_{e \in E_4} x^{3} + \sum_{e \in E_6} x^{4} = (9n^2 - 3n)x^3 + (6n)x^4
\]

Now, the first Zagreb index and Second Zagreb index of polycyclic aromatic hydrocarbon \( PAH_n \) will be

\[
Z_{g1}(PAH_n) = \left( \frac{\partial Z_{g1}(PAH_n,x)}{\partial x} \right)_{x=1}
\]

\[
= (9n^2 - 3n)x^2 + 6n \times 4n = 54n^2 + 6n
\]
Here, we complete the proof of Theorem 1. □

3. Conclusion

In this paper, we count two topological indices and their topological polynomials of a family of hydrocarbon molecular graphs "polycyclic aromatic hydrocarbon PAHx". These topological indices are useful for surveying the connected structure of these nanotubes, which have relation with degrees of its vertices.

References