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Research article

Hosoya, Schultz, Modified Schultz Polynomials and Their Topological Indices of *Benzene Molecules*: First Members of *Polycyclic Aromatic Hydrocarbons (PAHs)*

Mohammad Reza Farahani,

Department of Applied Mathematics,

Iran University of Science and Technology (IUST),

Narmak, Tehran 16844, Iran.

E-mail: MR_Farahani@mathdep.iust.ac.ir

MRFarahani88@gmail.com

Abstract

A topological index is a real number related to the structure of a connected graph G and is invariant under graph automorphism. Let G be a (molecular) graph possessing n vertices and m edges, and $e=x,y$ be an edge of G and x, y are two of its vertices, then the distance $d(x,y)=d(x,y|G)$ between the vertices x and y is equal to the length of the shortest path that connects them in G.

The goal of this paper is to compute the Schultz Polynomial $Sc(G,x)=\frac{1}{2}\sum_{\{u,v\}\subset V(G)}(d_u+d_v)x^{d(u,v)}$, Modified Schultz Polynomial $Sc^*(G,x)=\frac{1}{2}\sum_{\{u,v\}\subset V(G)}(d_u d_v)x^{d(u,v)}$, Hosoya Polynomial $H(G,x)=\frac{1}{2}\sum_{\{u,v\}\subset V(G)}x^{d(v,u)}$ and their topological indices of first members of a family of hydrocarbon structures "*Polycyclic Aromatic Hydrocarbons (PAHs)"* molecular graph.

Keywords: Polycyclic Aromatic Hydrocarbons (PAHs), Benzenoid, Topological Indices, Wiener Index, Hosoya Polynomial, Schultz Polynomial, Modified Schultz Polynomial.

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Introduction

Let *G=(V,E)* a simple finite molecular graph with the vertex set *V(G)* (the number of vertices *|V(G)|=n*) and the edge set *E(G)* (the number of vertices *|E(G)|=m*), such that in the connected molecular graph *G*, vertices represent atoms and edges represent bonds.

In graph theory, if *e* is an edge of G, connecting the vertices *u* and *v*, then we write *e=uv*. If G is a connected graph and *x* and *y* are two of its vertices, then the distance

*d(x,y)=d(x,y|*G*)* between the vertices *x* and *y* is equal to the length of the shortest path that connects them in G. Also the number of adjacent of vertex *v* is its degree, which denoted by d_v.

In chemical graph theory, we have invariant polynomials for any graphs, that they have usually integer coefficients. A topological index of *G* is a numeric quantity, derived following certain rules in Chemistry, which can be used to characterize the property of molecule.

Usage of topological indices in Biology and Chemistry began in 1947 when chemist *Harold Wiener* [1] introduced Wiener index to demonstrate correlations between physico-chemical properties of organic compounds of molecular graphs. The Wiener number is sum of distances between all unordered pairs of vertices of a simple graph *G*.

Also, for this topological index, the Hosoya polynomial was introduced by *H. Hosoya*, in 1988 [2]. The Wiener index *W(G)* and its polynomial (Hosoya) *H(G,x)* are define as follow:

$$W\left(G\right)=\frac{1}{2}\sum_{v\in V\left(G\right)}\sum_{u\in V\left(G\right)}d\left(v,u\right)$$

$$H\left(G,x\right)=\frac{1}{2}\sum_{v\in V\left(G\right)}\sum_{u\in V\left(G\right)}x^{d\left(v,u\right)}$$

Another based structure descriptors is the "*molecular topological index*" (Schultz index) was introduced by *Harry P. Schultz* in 1989 [3] and the Modified Schultz index was defined by *S. Klavžar* and *I. Gutman* in 1997 [4].

The Schultz index is defined as:

$$Sc\left(\mathrm{G}\right)=\frac{1}{2}\sum_{\{u,v\}\subset V\left(G\right)}(d_u+d_v)d(u,v)$$

where d_u and d_v are degrees of vertices *u* and *v*.

And the Modified Schultz polynomial of *G* is defined as:

$$Sc^{*}\left(\mathrm{G}\right)=\frac{1}{2}\sum_{\{u,v\}\subset V\left(G\right)}d(u,v)\left(d_u d_v\right)$$

Also for these One of the important, we have two important polynomials "*Schultz polynomial*" and "*Modified Schultz polynomial*". Schultz and Modified Schultz polynomials of *G* are defined respectively as:

$$Sc\left(\mathrm{G},\mathrm{x}\right)=\frac{1}{2}\sum_{\{u,v\}\subset V\left(G\right)}(d_u+d_v)x^{d(u,v)}$$

$$Sc^{*}(\mathrm{G},\mathrm{x})=\frac{1}{2}\sum_{\{u,v\}\subset V(G)}(d_u d_v)x^{d(u,v)}$$

These based structure descriptors and their polynomials studied and computed in many papers [3-15].

In this paper, we focus on the structure of first member of *Polycyclic Aromatic Hydrocarbons (PAHs)*, which called *Bezene* molecules. And formulas of its Hosoya, Schultz, Modified Schultz polynomials and their topological indices are determined for the first time.

Results and Discussion

In this section we compute Hosoya, Schultz and Modified Schultz polynomials, Wiener, Schultz and Modified Schultz indices of first members of *Polycyclic Aromatic Hydrocarbons* molecules, which called *Benzene* PAH_1 in Theorem1.

Polycyclic Aromatic Hydrocarbons PAHn is a family of hydrocarbon molecules, such that its structure is consisting of cycles with length six (*Benzene*).

In Refs [16-29] some properties and more historical details of this family of hydrocarbon molecules are studed. Also polycyclic aromatic hydrocarbons *PAHn* family are very similar properties to one of famous family of *Benzenoid* system (*Circumcoronene Homologous Series of Benzenoid* H_k). The properties and applications of Benzenoid system are presented in many papers; reader can see references [30-43].

Theorem 1. Let PAH_1 be the first members of *Polycyclic Aromatic Hydrocarbons (PAHs)*: "*Benzene* molecules". Then Hosoya, Schultz and Modified Schultz polynomials of PAH_1 are equal to

- $H(PAH_1,x)=12x^1+18x^2+21x^3+12x^4+3x^5$
- $SC(PAH_1,x)=60x^1+96x^2+78x^3+36x^4+6x^5$
- $SC^*(PAH_1,x)=72x^1+180x^2+69x^3+24x^{4+}3x^5$

And also the following topological indices of Benzene PAH_1 are calculated by formulas:

- Wiener index : $W(PAH_1)=164$
- Schultz index : $SC(PAH_1)=660$
- Modified Schultz index : $SC^*(PAH_1)=750$

Before prove the main theorem, we need the following denotations.

Denotation 1. Let $d(u,v)=i$ is distance between vertices u and v of G. Then, $D_i=\{(u,v)\,|\,u,v\in V(G), d(u,v)=i\}$ and we denoted the size of D_i by $d(G,i)$. Thus the diameter $d(G)$ is the longest topological distance in G.

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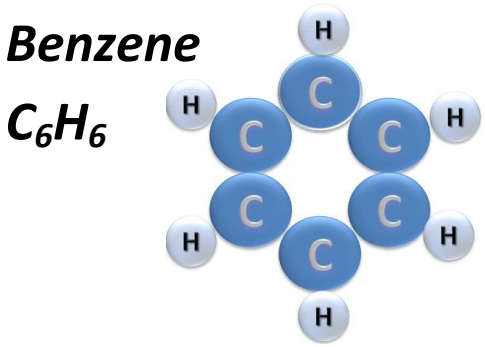

Figure 1. First member of of *Polycyclic Aromatic Hydrocarbons (PAHs)*: "*Benzene* molecules"

Proof of Theorem 1: Let $G=PAH_1$ be the *Benzene (*frist member of the polycyclic aromatic hydrocarbon family) with six carbon (C) and six hydrogen (H) atoms. Obviously we have the $\binom{12}{2}=66$ distinct shortest path between vertices/atoms u and v of G. So, from Figure 1, there are distances from one to five, for every vertices $u,v \in V(G)$.

In other words, $\forall u,v \in V(G), \exists d(u,v) \in \{1,2,3,4,5\}$ and obviously $|D_1|+|D_2|+|D_3|+|D_4|+|D_5|=66$. So, we will have five partitions for proof.

I. If $d(u,v)=1$, then $|D_1|=12$ and is equal to $|E(PAH_1)|$. So, we have three subsets of it.

I-1. For six carbon (C) atoms: $|D_1(C)|=|\{(u,v)|\ u,v \in V(PAH_1),\ d(u,v)=1\ \&\ d_u+d_v=6,\ d_u \times d_v=9\}|=6$. Therefore, we have three terms $6x^1$, $36x^1$, $54x^1$ of the Hosoya, Schultz and Modified Schultz polynomials, respectively.

I-2. For six hydrogen (H) atoms: $|D_1(H)|=|\{(u,v)|\ u,v \in V(PAH_1),\ d(u,v)=1\ \&\ d_u+d_v=4,\ d_u \times d_v=3\}|=6$. So, we have three sentences $6x^1$, $24x^1$ and $18x^1$ of the Hosoya, Schultz and Modified Schultz polynomials, respectively.

In general, we have three terms $12x^1$, $60x^1$ and $72x^1$ for of the above polynomials, respectively.

II. If $d(u, v)=2$, then $|D_2|=2\times 6_{CH}+1\times 6_{CC}=18$ and similarly, we have

II-1. For carbon atoms: $|D_2(C)|=|\{(u,v)|\ u,v \in V(PAH_1),\ d(u,v)=2\ \&\ d_u+d_v=6,\ d_u \times d_v=9\}|=12$. Hence, we have three terms $12x^2$, $72x^2$, $108x^2$ of the Hosoya, Schultz and Modified Schultz polynomials, respectively.

II-2. For hydrogen atoms: $|D_2(H)|=|\{(u,v)|\ u,v \in V(PAH_1),\ d(u,v)=2\ \&\ d_u+d_v=4,\ d_u \times d_v=3\}|=6$. Hence, we have three terms $6x^2$, $24x^2$, $18x^2$ of these above polynomials, respectively.

So generally, the second term of the Hosoya, Schultz and Modified Schultz polynomials are $18x^2$, $96x^2$ and $180x^2$, respectively.

III. If $d(u, v)=3$, then $|D_3|=1\times 6_{HH}+2\times 6_{CH}+3_{CC}=21$ and so, we have three subsets of it.

III-1. For carbon atoms: $|D_3(C)|=|\{(u,v)|u,v \in V(PAH_1),\ d(u,v)=3\ \&\ d_u+d_v=6,\ d_u \times d_v=9\}|=3$ and we have three terms $3x^3$, $18x^3$, $27x^3$ of the Hosoya, Schultz and Modified Schultz polynomials, respectively.

III-2. For hydrogen (H) atoms: $|D_3(H)|=|\{(u,v)|u,v \in V(PAH_1),\ d(u,v)=3\ \&\ d_u+d_v=2,\ d_u \times d_v=1\}|=6$. So, we have three sentences $6x^3$, $12x^3$ and $6x^3$ of the Hosoya, Schultz and Modified Schultz polynomials, respectively.

III-3. Finally for twelve paths between carbon and hydrogen atoms as distance 3, we have three terms $12x^3$, $48x^3$, $36x^3$ for the Hosoya polynomial, Schultz polynomial and Modified Schultz polynomial, respectively.

And generally, the thired sentence of the above polynomials are equale to $21x^3$, $78x^3$ and $69x^3$, respectively.

IV- If $d(u,v)=4$, then $|D_4|=1\times 6_{HH}+6_{CH}=9$ and we have two subsets of D_4 as

IV-1. For hydrogen (H) atoms: $|D_4(H)|=|\{(u,v)|u,v\in V(PAH_1),\ d(u,v)=4\ \&\ d_u+d_v=2,\ d_u\times d_v=1\}|=6$. Thus $6x^4$, $12x^4$ and $6x^4$ are in the Hosoya, Schultz and Modified Schultz polynomials, respectively.

IV-2. Similarly, for carbon atoms: $|D_4(C)|=|\{(u,v)|u,v\in V(PAH_1),\ d(u,v)=4\ \&\ d_u+d_v=4,\ d_u\times d_v=3\}|=6$ and we have three terms $6x^4$, $24x^4$ and $18x^4$, respectively.

Generally, we will have tow sentences $36x^4$ and $24x^4$ of the Schultz and Modified Schultz polynomials and $12x^4$ of the Hosoya polynomial.

V- If $d(u,v)=5$, then $|D_5|=|D_5(H)|=|\{(u,v)|u,v\in V(PAH_1),\ d(u,v)=5\ \&\ d_u+d_v=2,\ d_u\times d_v=1\}|=3$ and obviusly we have three terms $3x^5$, $6x^5$ and $3x^5$ for the Hosoya, Schultz and Modified Schultz polynomials of PAH_1, respectively.

Now, by enumerate all distinct shortest path between vertices/atoms u,v of *Benzene* PAH_1, its Hosoya polynomial is equal to:

$$H(PAH_1,x)=12x^1+18x^2+21x^3+12x^4+3x^5$$

And the Wiener index of *Benzene* PAH_1 is as follow:

$$W(PAH_1)=\frac{\partial H\left(PAH_1,x\right)}{\partial x}=12\times 1+18\times 2+21\times 3+12\times 4+3\times 5=164.$$

The Schultz polynomial of PAH_1 is equal to:

$$SC(PAH_1,x)=60x^1+96x^2+78x^3+36x^4+6x^5$$

And the Schultz index of PAH_1 is equal to:

$$SC(PAH_1)=\frac{\partial SC\left(PAH_1,x\right)}{\partial x}=60\times 1+96\times 2+78\times 3+36\times 4+6\times 5=660$$

Finally, the Modified Schultz polynomial and Modified Schultz index of PAH_1 are equale to:

$$SC^*(PAH_1,x)=72x^1+180x^2+69x^3+24x^{4+}3x^5$$

And also,

$$SC^*(PAH_1)=\frac{\partial SC^*\left(PAH_1,x\right)}{\partial x}=72\times 1+180\times 2+69\times 3+24\times 4+3\times 5=750$$

Here, we complete the proof of Theorem 1. □

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