Research article

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

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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 $S_c(G,x)=\frac{1}{2} \sum_{(x,y) \in V(G)} (d_x + d_y)x^{d(x,y)}$, Modified Schultz Polynomial $S_{c'}(G,x)=\frac{1}{2} \sum_{(x,y) \in V(G)} (d_x d_y)x^{d(x,y)}$, Hosoya Polynomial $H(G,x)=\frac{1}{2} \sum_{(x,y) \in V(G)} x^{d(x,y)}$ and their topological indices of first members of a family of hydrocarbon structures “Polycyclic Aromatic Hydrocarbons (PAHs)” molecular graph. Copyright © acascipub.com, all rights reserved.

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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:

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

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

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:

$$Sc(G) = \frac{1}{2} \sum_{(u,v) \in E(G)} (d_u + d_v)d(u,v)$$

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

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

$$Sc^*(G) = \frac{1}{2} \sum_{(u,v) \in E(G)} d(u,v)(d_u d_v)$$

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:

$$Sc(G,x) = \frac{1}{2} \sum_{(u,v) \in E(G)} (d_u + d_v)x^{d(u,v)}$$
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 Benzene 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 PAH₁ in Theorem 1.

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 studied. Also polycyclic aromatic hydrocarbons PAHₙ family are very similar properties to one of famous family of Benzenoid system (Circumcoronene Homologous Series of Benzenoid Hₖ). The properties and applications of Benzenoid system are presented in many papers; reader can see references [30-43].

**Theorem 1.** Let PAH₁ be the first members of Polycyclic Aromatic Hydrocarbons (PAHs): “Benzene molecules”. Then Hosoya, Schultz and Modified Schultz polynomials of PAH₁ are equal to

- \[ H(PAH₁,x)=12x^1+18x^2+21x^3+12x^4+3x^5 \]
- \[ SC(PAH₁,x)=60x^1+96x^2+78x^3+36x^4+6x^5 \]
- \[ SC^*(PAH₁,x)=72x^1+180x^2+69x^3+24x^4+3x^5 \]

And also the following topological indices of Benzene PAH₁ are calculated by formulas:

- Wiener index : \[ W(PAH₁)=164 \]
- Schultz index : \[ SC(PAH₁)=660 \]
- Modified Schultz index : \[ SC^*(PAH₁)=750 \]

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 \( G \).
Proof of Theorem 1: Let $G=PAH_1$ be the Benzene (first 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: $|D_1(C)|=|\{(u,v)|u,v \in V(PAH_1), \ d(u,v)=1 \wedge d_u+d_v=6, \ d_u \times d_v=9\}|=6$. 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: $|D_1(H)|=|\{(u,v)|u,v \in V(PAH_1), \ d(u,v)=1 \wedge d_u+d_v=4, \ d_u \times d_v=3\}|=6$. Hence, 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 $|D_2|=2\times6_{CH}+1\times6_{CC}=18$ and similarly, we have

II-1. For carbon atoms: $|D_2(C)|=|\{(u,v)|u,v \in V(PAH_1), \ d(u,v)=2 \wedge d_u+d_v=6, \ d_u \times d_v=9\}|=12$. 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: $|D_2(H)|=|\{(u,v)|u,v \in V(PAH_1), \ d(u,v)=2 \wedge d_u+d_v=4, \ d_u \times d_v=3\}|=6$. 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 $|D_3|=1\times6_{HH}+2\times6_{CH}+3_{CC}=21$ and so, we have three subsets of it.

III-1. For carbon atoms: $|D_3(C)|=|\{(u,v)|u,v \in V(PAH_1), \ d(u,v)=3 \wedge d_u+d_v=6, \ d_u \times d_v=9\}|=3$ 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: $|D_3(H)|=|\{(u,v)|u,v \in V(PAH_1), \ d(u,v)=3 \wedge d_u+d_v=2, \ d_u \times d_v=1\}|=6$. 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 third sentence of the above polynomials are equal to $21x^3$, $78x^3$ and $69x^3$, respectively.

IV- If $d(u,v)=4$, then $|D_4|=l_{HVV}+6CH=9$ 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 two 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 obviously 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:

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

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:

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

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

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

And also,

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

Here, we complete the proof of Theorem 1. □
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