SOME COMPUTATIONAL ASPECTS OF N-PYRENE USING CERTAIN DEGREE BASED TOPOLOGICAL INDICES AND THEIR M POLYNOMIALS

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ABSTRACT

In this article, we first summarized the graph invariants and derive the M-polynomial of *n*-pyrene. Here, we focus on the structure of pyrene polycyclic aromatic hydrocarbons PAH_2 and we draft some general expression for discrete invariant polynomials and some connectivity indices like Randic index, Zagreb indices.

KEYWORDS

Graph Invariant, Topological indices, Invariant polynomials, *n*-pyrene, Subdivision graph, Semi-total point graph.

1. Introduction

Pyrene is Polycyclic Aromatic Hydrocarbon, consisting four fused benzene rings, resulting in a flat aromatic system. The molecular formula is $C_{16}H_{10}$. It has no colour and it is represented as a solid which is the smallest peri-fused *PAH*.Pyrene was first isolated from coal tar, where it occurs up to 2 percentages by weight. *PAHs* are created when products like coal, oil, gas and garbage is burned but the burning process is not complete.

Molecular graph is used to represent the structural formula of a chemical compound, its vertices being atoms and edges corresponding to covalent bonds in the molecules. Usually it is hydrogen depleted molecular graph

The following graph is the hydrogen depleted molecular graph of pyrene:

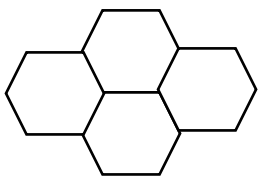

Fig 1: Molecular graph of pyrene

n-pyrene is a polycyclic aromatic hydrocarbon containing *n* fused benzene rings at one side, the graphical structure of *n*-pyrene is obtained by taking *n* number of pyrene as chain

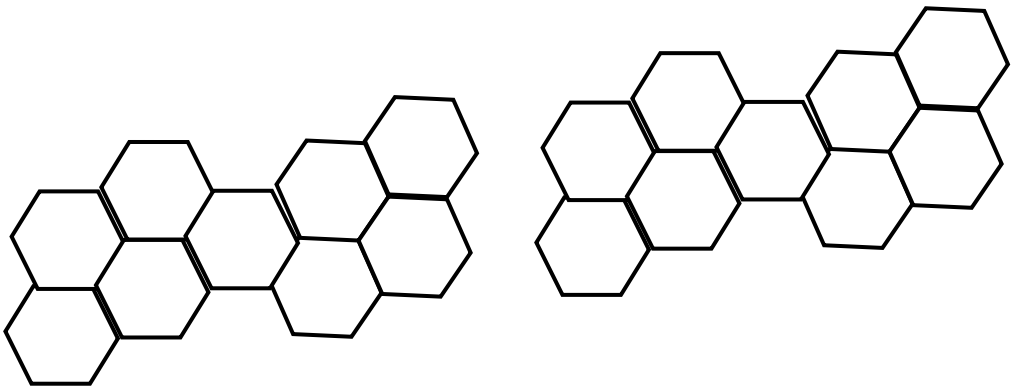

Fig 2: Molecular graph of *n*-pyrene

In chemical graph theory, we have invariant polynomial and topological indices for any molecular graphs, such that topological indices of molecular graphs and nano structure are numerical descriptors that are derived from the graph of chemical compounds, such indices based on the degree of graph are widely used for establishing relationship between the structure of molecular graphs and their physiochemical properties.

A graph invariant is a property which is preserved by isomorphism. In other words, a graph invariant is a property which must be same for any two isomorphic graphs. Graph invariant depends only on the abstract structure, not on graph representations such as particular labeling or drawings of the graph.

A topological index which is also called as molecular descriptor is a mathematical formula that can be applied to any graph which models the molecular structure. The purpose of defining a topological index is to represent each chemical structure with a numerical value. By this index it is possible to analyze mathematical values and further investigate some physiochemical properties of a molecule. Therefore, it is an efficient method in avoiding expensive and time-consuming laboratory experiments. For more information on the topological indices may refer[**15-16]**

2. Essential prerequisite

Let G be a graph and d_u is a degree of vertex $u \in V(G)$ and $uv \in E(G)$ is the edge. In this section we recall some essential definitions and discuss prerequisites which are used in development of this article.

Definition 2.1: The **Subdivision graph [1]** $S(G)$ is the graph obtained by replacing each of its edge by a path of length 2 or equivalently, by inserting an additional vertex into each edge of G.

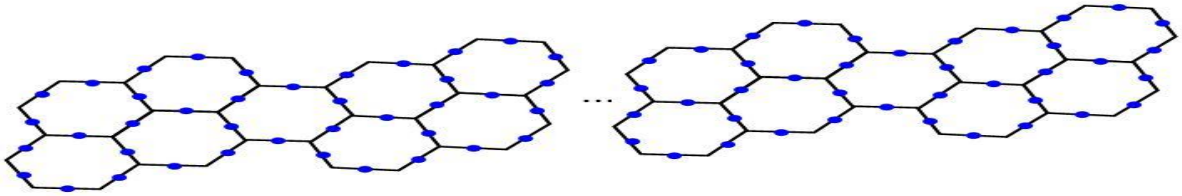

Fig 3: Subdivision graph of n-pyrene

Definition2.2: The **Semi total point graph [14]** *ST(G)* is the graph obtained from *G* by adding a new vertex corresponding to each edge of *G* and by joining each new vertex to the end vertex of edge corresponding to it

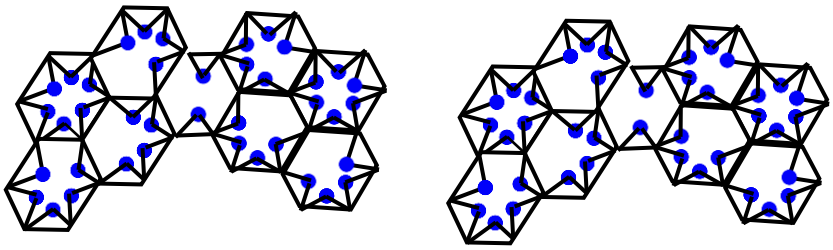

Fig 4: semi total point graph of n-pyrene

D. Vukicevic [8-9] notified the 148 discrete adriatic indices. They were analyzed on the testing sets provided by the International Academy of Mathematical Chemistry and it had been shown that they have good presaging properties in many cases. We discuss some of them in this paper.

Definition 2.3: The **First and Second Zagreb indices** were introduced more than thirty years ago by **Gutman** and **Trinajstic [10]** which are defined as

$$M_1(G) = \sum_{uv \in E(G)} d_u + d_v \text{ and } M_2(G) = \sum_{uv \in E(G)} d_u d_v$$

Both first Zagreb index and the second Zagreb index give greater weights to the inner vertices and edges and smaller weights to the outer vertices and edges, which opposes intuitive reasoning

The **Second Modified Zagreb index [11]** is defined as

$${}^{m}M_2(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v}$$

Definition 2.4: The **Randic [12] index** denoted by *R(G)* and introduced by Milan Randic in 1975 is also one of the oldest topological index and is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

In 1998, working independently, **Bollobas and Erdos [3]** and **Amicet. Al., [2]** proposed the generalized Randi'c index and has been studied extensively by both chemists and mathematicians. The **Ordinary Randic connectivity index** has been extended to the general Randic connectivity index defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$$

Definition 2.5: The **M-polynomial of a graph G** is defined as

$$M(G; x, y) = \sum_{i \le j} m_{ij}(G) x^i y^j$$

Where $m_{ij}(G)$, *(i, j≥1)* be the number of edges *e=uv* of Gsuch that $(d_u, d_v) = (i, j)$

Table 1.**Derivation of some degree-based topological indices from M-polynomial**

Topological index	***f(x,y)***	**Derivation from M(G;x,y)**
First Zagreb	$x+y$	$(D_x + D_y)(M(G;x,y))\|_{x=y=1}$
Second Zagreb	xy	$(D_x D_y)(M(G;x,y))\|_{x=y=1}$
Second Modified Zagreb	$\frac{1}{xy}$	$(S_x S_y)(M(G;x,y))\|_{x=y=1}$
Generalized Randic	$(xy)^{\alpha}$	$(D_x^{\alpha} D_y^{\alpha})(M(G;x,y))\|_{x=y=1}$

Where

$$D_x = x\frac{\partial(f(x,y))}{\partial x}, \quad D_y = y\frac{\partial(f(x,y))}{\partial y}, \; S_x = \int_0^x \frac{f(t,y)}{t}dt, \; S_x = \int_0^y \frac{f(x,t)}{t}dt,$$

3. Main Results

In this section, we present our main results. In the following we determine the topological indices and M-polynomial of *n*-pyrene.

The Graphical structure of *n*-pyrene is represented in the **Fig 2**. The graph of *n*-pyrene has np vertices and $nq+2(n-1)$ edges, where *p=16, q=19*and *n=1, 2, 3…*

Table 2. The edge partition of *n*-pyrene based on degree of end vertices of each edge.

(d_u, d_v)	**Number of edges**
(2,2)	$2n+4$
(2,3)	$8n$
(3,3)	$11n-6$

Table 3. The edge partition of subdivision graph of n-pyrene based on degree of end vertices of each edge.

(d_u, d_v)	**Number of edges**
(2,2)	$11n+9$
(2,3)	$31n-13$

Table 4. The edge partition of semi total point graph of n-pyrene based on degree of end vertices of each edge.

(d_u, d_v)	**Number of edges**
(2,4)	$10n+11$
(2,6)	$34n-17$
(4,4)	$2n+4$
(4,6)	$8n$
(6,6)	$9n-4$

Theorem 3.1: Let G be a graph of n-pyrene and n=1,2, 3… then the M-polynomial is

$$M(G;x,y)=(2n+4)x^2y^2+8nx^2y^3+(11n-6)x^3y^3.$$

Proof: Consider a graph of n-pyrene then from **Fig 2,** we have,

$$|V(G)|=np,$$
$$|E(G)|=nq+2(n-1),$$

The edge set of G can be partitioned into 3 sets based on the degree of end vertices.

$$E_{2,2}=\{uv\in E(G)/d_u=2,d_v=2\},$$
$$E_{2,3}=\{uv\in E(G)/d_u=2,d_v=3\},$$
$$E_{3,3}=\{uv\in E(G)/d_u=3,d_v=3\},$$

From **Table 2,** we have,

$$|E_{(2,2)}|=2n+4,$$
$$|E_{(2,3)}|=8n,$$
$$|E_{(3,3)}|=11n-6,$$

Thus the M-polynomial of *n*-pyrene is,

$$M(G;x,y)=\sum_{i\le j} m_{ij}(G)x^iy^j$$

$$=\sum_{i=j=2} m_{22}(G)x^2y^2+\sum_{2\le 3} m_{23}(G)x^2y^3+\sum_{i=j=3} m_{33}(G)x^3y^3$$

$$=|E_{(2,2)}|x^2y^2+|E_{(2,3)}|x^2y^3+|E_{(3,3)}|x^3y^3$$

$$M(G;x,y)=(2n+4)x^2y^2+8nx^2y^3+(11n-6)x^3y^3.$$

Theorem 3.2: Let G be the graph of n-pyrene and n=1, 2, 3,…, then

1. $M_1(G) = 114n - 20$
2. $M_2(G) = 155n - 38$
3. $M_2^m(G) = \frac{n+2}{2} + \frac{4n}{3} + \frac{11n-6}{6}$
4. $R_\alpha(G) = 2^{\alpha+1}n + 2^{2\alpha+2} + 3^\alpha 2^{\alpha+3}n + 3^{2\alpha}11n - 2.3^{2\alpha+1}$.

Proof: The required results are obtained by substituting **Table 1** results into the M-polynomial of n-pyrene.

Theorem 3.3: Let H be the subdivision graph of n-pyrene. Then the M-polynomial of H is

$$\mathrm{M}(H,x,y) = (11n+9)x^2y^2 + (31n-13)x^3y^3$$

Proof: Consider the subdivision graph of n-pyrene as shown in **Fig 3 .**

The edge set of H can be partitioned into 2 sets based on the degree of end vertices,

$$E_{2,2} = \{uv \in E(G) / d_u = 2, d_v = 2\},$$
$$E_{2,3} = \{uv \in E(G) / d_u = 2, d_v = 3\},$$

From **Table 3** we have,

$$|E_{(2,2)}| = 11n+9,$$

$$|E_{(2,3)}| = 31n-13,$$

Thus the M-polynomial of Subdivision graph of *n*-pyrene is,

$$M(H;x,y) = \sum_{i\le j} m_{ij}(H)x^i y^j$$

$$= \sum_{i=j=2} m_{22}(H)x^2y^2 + \sum_{2\le 3} m_{23}(H)x^2y^3$$

$$= |E_{(2,2)}|\, x^2y^2 + |E_{(2,3)}|\, x^2y^3$$

$$\mathrm{M}(H,x,y) = (11n+9)x^2y^2 + (31n-13)x^3y^3.$$

Theorem 3.4: Let H be the Subdivision graph of *n*-pyrene and n=1, 2, 3 … then

1. $M_1(H) = 199n + 21$
2. $M_2(H) = 230n + 18$
3. $M_2^m(H) = \frac{95n}{12} + \frac{7}{4}$
4. $R_\alpha(H) = 2^{\alpha+1}(11n+9) + 3^\alpha 2^\alpha(31n-3)$.

Proof: The required results are obtained by substituting **Table 1** resultsinto the M-polynomial of subdivision graph of *n*-pyrene.

Theorem 3.5: Let P be a Semi total point graph of *n*-pyrene and n=1,2,3 … then the M-polynomial of P is

$$M(P;x,y) = (10n+11)x^2y^4 + (34n-17)x^2y^6 + (2n+4)x^4y^4 + (8n)x^4y^6 + (9n-4)x^6y^6$$

Proof: Consider the Semi total point graph of n-pyrene as shown in **Fig 4**.

The edge set of P can be partitioned into 5 sets based on the degree of end vertices,

$$E_{2,4} = \{uv \in E(P) / d_u = 2, d_v = 4\},$$
$$E_{2,6} = \{uv \in E(P) / d_u = 2, d_v = 6\},$$
$$E_{4,4} = \{uv \in E(P) / d_u = 4, d_v = 4\},$$
$$E_{4,6} = \{uv \in E(P) / d_u = 4, d_v = 6\},$$
$$E_{6,6} = \{uv \in E(P) / d_u = 6, d_v = 6\},$$

From **Table 4** we have,

$$|E_{(2,4)}| = 10n+11,$$
$$|E_{(2,6)}| = 34n-17,$$
$$|E_{(4,4)}| = 2n+4,$$
$$|E_{(4,6)}| = 8n,$$
$$|E_{(6,6)}| = 9n-4.$$

Thus, the M-polynomial of Semi total point graph of *n*-pyrene is,

$$M(P;x,y) = \sum_{i\le j} m_{ij}(P)x^i y^j$$
$$= \sum_{2\le 4} m_{24}(P)x^2y^4 + \sum_{2\le 6} m_{26}(P)x^2y^6 + \sum_{i=j=4} m_{44}(P)x^4y^4 + \sum_{4\le 6} m_{46}(P)x^4y^6 + \sum_{i=j=6} m_{66}(P)x^6y^6$$
$$= |E_{(2,4)}|x^2y^4 + |E_{(2,6)}|x^2y^6 + |E_{(4,4)}|x^4y^4 + |E_{(4,6)}|x^4y^6 + |E_{(6,6)}|x^6y^6$$

$$M(P;x,y) = (10n+11)x^2y^4 + (34n-17)x^2y^6 + (2n+4)x^4y^4 + (8n)x^4y^6 + (9n-4)x^6y^6$$

Theorem 3.6: Let P be a Semi total point graph of *n*-pyrene and *n*=1,2,3 … then

1. $M_1(P) = 352n - 86$
2. $M_2(P) = 1036n - 196$
3. $M_2^m(P) = \frac{115n}{24} - \frac{7}{72}$

4. $R_\alpha(P) = (10n+11)2^{3\alpha} + (34n-17)2^\alpha 6^\alpha + (2n+4)2^{4\alpha} - (8n)2^{2\alpha}6^\alpha + (9n-4)6^{2\alpha}$.

Proof: The required results are obtained by substituting **Table 1** results into the M-polynomial of Semi total point graph of *n*-pyrene

4. Conclusion

In this article, we have obtained the M-polynomial for n-pyrene, subdivision graph and semi total point graph of *n*-pyrene by using the method of edge partitions. The Topological indices thus obtained are helpful to study QSAR and QSPR properties of these molecular structures, that is to understand the physical feature, chemical reactivity and biological activities. The topological index is considered as vital role that maps each molecular structure to a real number

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