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SOME COMPUTATIONAL ASPECTS OF LINEAR CHAIN OF ANTHRACENE USING CERTAIN DEGREE BASED TOPOLOGICAL INDICES AND THEIR M POLYNOMIALS

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ABSTRACT. In this article, we have summarized the graph invariants and derived the M-polynomial of linear[n]-anthracene. Here, focus has been drawn on the structure of anthracene polycyclic aromatic hydrocarbons and we draft some general expression for discrete invariant polynomials with various indices like Zagreb indices, Randic index, Inverse randic index, Harmonic index, symmetric division degree index and Inverse sum index.

1. Introduction

Anthracene is a solid polycyclic aromatic hydrocarbon (PAH) with the molecular formula $C_{14}H_{10}$, consisting of three fused benzene rings. Also referred to as para-naphthalene or green oil, it is the simplest tricyclic aromatic hydrocarbon and occurs naturally in coal tar. Classified as a priority pollutant by the Environmental Protection Agency (EPA), anthracene is a byproduct of the incomplete combustion of fossil fuels and is widely dispersed in the environment. It has been detected in various sources, including surface and drinking water, ambient air, vehicle exhaust, tobacco smoke, smoked foods, and aquatic organisms. The molecular structure of anthracene can be represented as a graph, where vertices correspond to atoms and edges represent covalent bonds, often excluding hydrogen atoms to simplify the depiction.

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

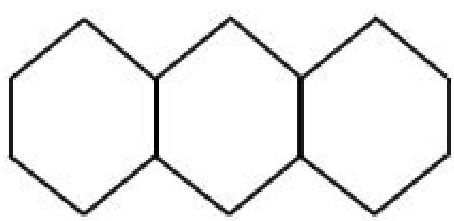

Fig 1: Molecular graph of anthracene.

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

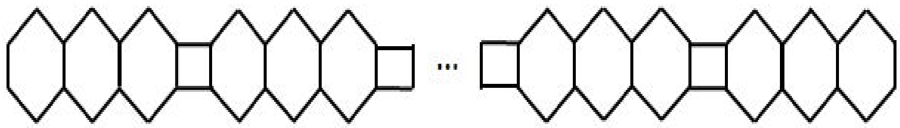

Fig 2: Molecular graph of linear[n]-anthracene.

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 further information on the topological indices may refer [7, 8]

Definition of subdivision graph and semi total point graph are found in [2, 7].

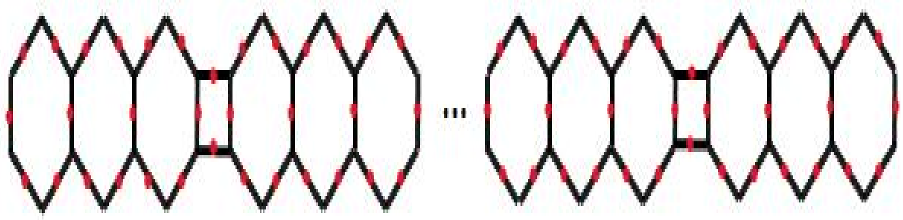

Fig 3: subdivision graph of linear[n]-anthracene.

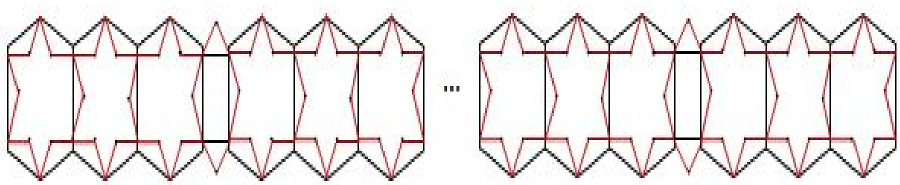

Fig 4: semi-total point graph of linear[n]-anthracene.

In this article we have considered following topological indices namely,
first and Second Zagreb indices[6] are defined as

$$M_1(G) = \sum_{pq \in E(G)} [d_p + d_q] \quad \text{and} \quad M_2(G) = \sum_{pq \in E(G)} d_p d_q.$$

The second modified Zagreb index [9] is defined as

$$^{m}M_2(G) = \sum_{pq \in E(G)} \frac{1}{d_p d_q}$$

For a connected graph G, symmetric division degree index [5, 4] is given by

$$SDD(G) = \sum_{pq \in E(G)} \frac{d_p^2 + d_q^2}{d_p d_q}$$

One of the earliest topological indices is the Randic index [10] and it was first presented by Milan Randic in 1975. It is described as

$$R(G) = \sum_{pq \in E(G)} \frac{1}{\sqrt{d_p d_q}}$$

In 1998, working independently, Bollobas and Erdos [3] and Amic et. al., [1] proposed the generalized Randic 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 and is defined as

$$R_\alpha(G) = \sum_{pq \in E(G)} (d_p d_q)^\alpha$$

The Inverse sum index [12] (ISI) is defined as

$$ISI(G) = \sum_{pq \in E(G)} \frac{d_q}{d_p + d_q}$$

The Harmonic index [11] is an additional Randic index variant that is described as

$$H(G) = \sum_{pq \in E(G)} \frac{2}{d_p + d_q}$$

M polynomial of a graph G [12] is defined as

$$M(G; s, t) = \sum_{i \leq j} n_{ij}(G) s^i t^j$$

here, $n_{ij}(G), (i, j \geq 1)$ gives count of edges $e = pq$ which has following property $(i, j) = (d_p, d_q)$.

Table 1.Some degree-based topological indices are generated using the M-polynomial.

Molecular discriptor	g(s,t)	An implication from M(G;s,t)
First Zagreb index	$s+t$	$(D_s+D_t)\,M(G;\text{s,t})\vert_{s=t=1}$
Second Zagreb index	st	$(D_sD_t)\,M(G;\text{s,t})\vert_{s=t=1}$
Second Modified Zagreb index	$\frac{1}{st}$	$(S_sS_t)M(G;\text{s,t})\vert_{s=t=1}$
Randic index	$(st)^{\alpha}$	$(D_s^{\alpha}D_t^{\alpha})\,M(G;\text{s,t})\vert_{s=t=1}$
Symmetric Division degree index	$\dfrac{s^{\alpha}+t^{\alpha}}{st}$	$(D_sS_t+S_sD_t)\,M(G;\text{s,t})\vert_{s=t=1}$
Harmonic index	$\frac{2}{s+t}$	$(2S_sJ)M(G;\text{s,t})\vert_{s=t=1}$
Inverse sum index	$\dfrac{st}{s+t}$	$(S_sJD_sD_t)M(G;\text{s,t})\vert_{s=t=1}$

where,

$$D_sg(s,t)=s\frac{\partial(g(s,t))}{\partial s}$$

$$D_tg(s,t)=t\frac{\partial(g(s,t))}{\partial t}$$

$$S_sg(s,t)=\int_0^s\frac{g(x,t)}{x}dx$$

$$S_tg(s,t)=\int_0^t\frac{g(s,y)}{y}dy$$

$$Jg(s,t)=g(s,s)$$

2. Main results

Our primary findings are presented in this section. Fig. 2 depicts the graphical structure of linear[n]-anthracene. The linear[n]-anthracene graph contains $14n$ vertices and $18(n-2)$ edges, where $n=1,2,3$.

Table 2. Linear[n]-anthracene's edge partition according to each edge's degree of end vertices.

(d_p, d_q)	(2,2)	(2,3)	(3,3)
Count of edges	6	12n-4	6n-4

Table 3. The subdivision graph of linear[n]-anthracene's edge partition is determined by the degree of each edge's end vertices.

(d_p, d_q)	(2,2)	(2,3)
Count of edges	12n+8	24n-12

Table 4. The semi-total point graph of linear[n]-anthracene's edge partition according to the degree of each edge's end vertices.

(d_p, d_q)	(2,4)	(2,6)	(4,4)	(4,6)	(6,6)
Count of edges	12n+8	24n-12	6	12n-4	6n-4

Theorem 2.1. *Let $n = 1, 2, 3, ...$ and G be a graph of linear[n]-anthracene, then closed form of M-polynomial is*

$$M(G; s, t) = 6s^2t^2 + (12n - 4)t^2t^3 + (6n - 4)s^3t^3.$$

Proof. As shown in Fig 2, linear[n]-anthracene has $14n$ vertices and $18n-2$ edges.

Depending on the degree of each edge's end vertices, the edge set can be divided into the following three sets.
$L_{2,2} = \{pq \in E(G)|d_p = 2, d_q = 2\}$
$L_{2,3} = \{pq \in E(G)|d_p = 2, d_q = 3\}$
$L_{3,3} = \{pq \in E(G)|d_p = 3, d_q = 3\}$.

we have, From Table 2
$|L_{2,2}| = 6$
$|L_{2,3}| = 12n - 4$
$|L_{3,3}| = 6n - 4$.
Hence, M polynomial of linear[n]-anthracene is

$$\begin{aligned} M(G; s, t) &= \sum_{i \leq j} n_{ij}(G)s^it^j \\ &= |L_{2,2}|\, s^2t^2 + |L_{2,3}|\, s^2t^3 + |L_{3,3}|\, s^3t^3 \\ &= 6s^2t^2 + (12n - 4)\, s^2t^3 + (6n - 4)\, s^3t^3. \end{aligned}$$

□

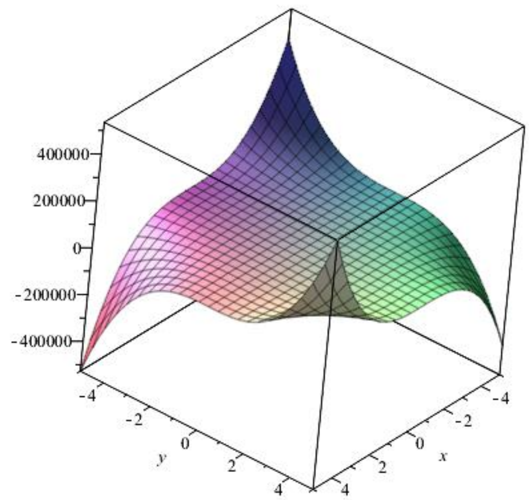

Fig 5: 3D plot of M-polynomial of linear[n]-anthracene for $n = 10$

Theorem 2.2. *If Gis the linear[n]-anthracene graph, where n is 1, 2, 3,..., then*
1. $M_1(G) = 96n - 20$
2. $M_2(G) = 126n - 36$
3. ${}^{m}M_2(G) = \dfrac{48n - 23}{18}$
4. $SDD(G) = 38n - \dfrac{14}{3}$
5. $H(G) = \dfrac{102n + 1}{15}$
6. $ISI(G) = \dfrac{117n - 24}{5}$
7. $R_\alpha(G) = 2^{2\alpha+1}3 + 2^{\alpha+2}3^{\alpha+1}n + 3^{2\alpha+1}2n - 2^{\alpha+2}3^{\alpha} - 3^{2\alpha}4.$

Proof. The M-polynomial of linear[n]-anthracene is substituted with the results from Table 1 to obtain the necessary results. □

Theorem 2.3. *If H is a linear[n]-anthracene subdivision graph, then its M-polynomial is*

$$M(H; s, t) = (12n + 8)s^2t^2 + (24n - 12)s^2t^3.$$

Proof. According to Fig. 3, The linear[n]-anthracene subdivision graph has $32n-2$ vertices and $36n - 4$ edges, respectively.

Based on the degree of each edge's end vertices, the edge set can be divided into the next two sets.
$L_{2,2} = \{pq \in E(H) | d_p = 2, d_q = 2\}$
$L_{2,3} = \{pq \in E(H) | d_p = 2, d_q = 3\}$

From the results of Table 3, we have
$|L_{2,2}| = 12n + 8$
$|L_{2,3}| = 24n - 12$

Hence, closed form of M polynomial of subdivision graph of linear[n]-anthracene is as follows

$$\begin{aligned} M(H; s, t) &= \sum_{i \leq j} n_{ij}(H) s^i t^j \\ &= |L_{2,2}|\, s^2 t^2 + |L_{2,3}|\, s^2 t^3 \\ &= (12n + 8)\, s^2 t^2 + (24n - 12)\, s^2 t^3. \end{aligned}$$

□

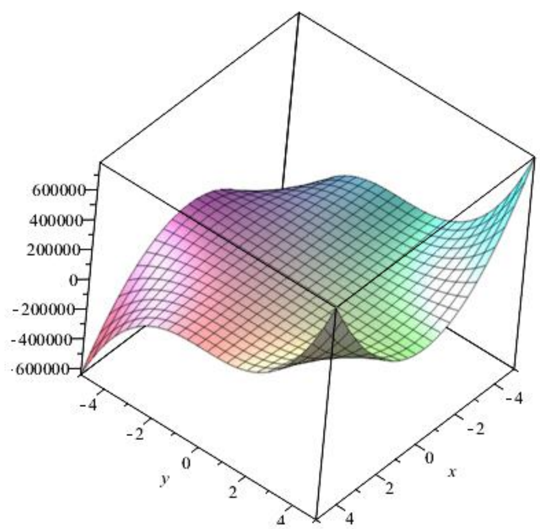

Fig 6: For $n = 10$, the 3D plot of M-polynomial of the subdivision graph of linear[n]-anthracene

Theorem 2.4. *Let H be the subdivision graph of linear[n]-anthracene then*
1. $M_1(H) = 168n - 28$
2. $M_2(H) = 192n - 32$
3. ${}^mM_2(H) = 7n$
4. $SDD(H) = 76n - 10$
5. $H(H) = \dfrac{156n - 8}{10}$
6. $ISI(H) = \dfrac{204n - 32}{5}$
7. $R_\alpha(H) = 2^{2\alpha+2}3n + 2^{2\alpha+3} + 2^{\alpha+3}3^{\alpha+1}n - 2^{\alpha+2}3^{\alpha+1}$.

Proof. The M-polynomial of the subdivision graph of linear[n]-anthracene is substituted with the results from Table 1 to obtain the necessary results.

□

Theorem 2.5. *If P is a linear[n]-anthracene semi-total point graph, then closed form of M-polynomial is*

$M(P;s,t) = (12n+8)s^2t^4 + (24n-12)s^2t^6 + 6s^4t^4 + (12n-4)s^4t^6 + (6n-4)s^6t^6.$

Proof. According to Fig 4, the semi-total point graph of linear[n]-anthracene has $32n-2$ vertices and $54n-6$ edges.

The degree of each edge's end vertices can be used to partition the edge set into the following five sets.
$L_{2,4} = \{pq \in E(P)|d_p = 2, d_q = 4\}$
$L_{2,6} = \{pq \in E(P)|d_p = 2, d_q = 6\}$
$L_{4,4} = \{pq \in E(P)|d_p = 4, d_q = 4\}$
$L_{4,6} = \{pq \in E(P)|d_p = 4, d_q = 6\}$
$L_{6,6} = \{pq \in E(P)|d_p = 6, d_q = 6\}$

Table 4 gives us following values,
$|L_{2,4}| = 12n+8$
$|L_{2,6}| = 24n-12$
$|L_{4,4}| = 6$
$|L_{4,6}| = 12n-4$
$|L_{6,6}| = 6n-4$

Formula of M polynomial of semi-total point graph of linear[n]-anthracene is

$$\begin{aligned} M(P;s,t) &= \sum_{i\leq j} n_{ij}(G)s^it^j \\ &= |L_{2,4}|\, s^2t^4 + |L_{2,6}|\, s^2t^6 + |L_{4,4}|\, s^4t^4 + |L_{4,6}|\, s^4t^6 + |L_{6,6}|\, s^6t^6 \\ &= (12n+8)\, s^2t^4 + (24n-12)\, s^2t^6 + (6)\, s^4t^4 + (12n-4)\, s^4t^6 + (6n-4)\, s^6t^6. \end{aligned}$$

□

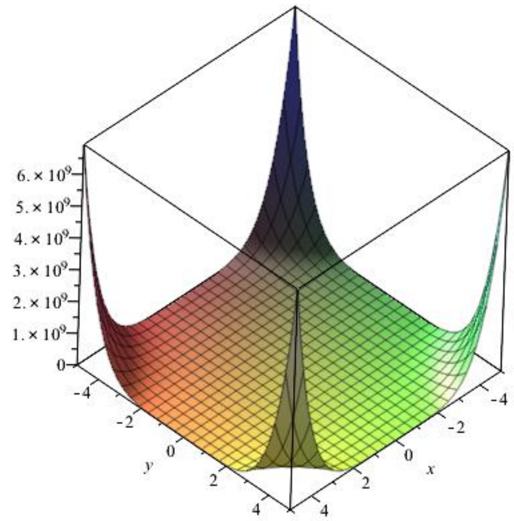

Fig 7: 3D plot of M-polynomial of linear[n]-anthracene's semi-total point graph for $n = 10$

Theorem 2.6. *Assuming that P is the linear[n]-anthracene semi-total point graph, then 1.* $M_1(P) = 456n - 88$
2. $M_2(P) = 888n - 224$
3. ${}^mM_2(P) = \frac{25n}{6} + \frac{7}{72}$
4. $SDD(P) = 148n - \frac{74}{3}$
5. $H(P) = \frac{134n - 3}{10}$
6. $ISI(P) = \frac{1482n - 254}{15}$
7. $R_\alpha(P) = 2^{3\alpha+2}3n + 2^{3\alpha+3} + 2^{2\alpha+3}3^{\alpha+1}n - 2^{2\alpha+2}3^{\alpha+1} + 2^{4\alpha+1}3 + 2^{3\alpha+2}3^{\alpha+1}n - 2^{3\alpha+2}3^{\alpha} + 2^{2\alpha+1}3^{2\alpha+1}n - 2^{2\alpha+2}3^{2\alpha}$.

Proof. To obtain the necessary results, the M-polynomial of the semi-total point graph of linear[n]-anthracene is substituted with the results from Table 1. □

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