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# CALCULATING DEGREE BASED TOPOLOGICAL INDICES OF LINE GRAPH OF $HAC_5C_6C_7[p, q]$ NANOTUBE VIA M-POLYNOMIAL

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Abstract. The application of graph theory in chemical and molecular structure research far exceeds people's expectations, and it has recently grown exponentially. In the molecular graph, atoms are represented by vertices and bonded by edges. In this report, we study the M-polynomial of line graph of $HAC_5C_6C_7[p, q]$ and recover many degree-based topological indices from it.
*Key words and phrases:* Line graph; Zagreb index; Molecular graph; Nanotube.

## 1. Introduction

Graph theory provides chemists with a variety of useful tools, such as topological indices. Molecular compounds are often modeled using molecular graphs. The molecular graph represents the structural formula of the compound in the form of graph theory, the vertices of which correspond to the atoms of the compound and the edges correspond to the chemical bonds [1].
Chemical informatics is a new area of research that integrates chemistry, mathematics, and information science. It studies the quantitative structure-activity (QSAR) and structure-property (QSPR) relationships [2, 3, 4, 5] used to predict the biological activity and properties of compounds. In the QSAR / QSPR study, the physical and chemical properties and topological indices such as Szeged index, Wiener index, Randi'c index, ABC index and Zagreb index etc were used to predict the biological activity of compounds. A molecular graph can be identified by topological index, polynomials, sequences or matrices [6].

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The topological index is a number associated with the graph [7]. It represents the topological structure of the graph and is invariant under the automorphism of the graph. There are some major topological index categories, such as distance-based topological indices [8, 9], degree-based topological indices [10, 11], and counting-related polynomial and graph indices [7]. In these categories, the degree-based topological index is very important and plays a crucial role in chemical graph theory, especially in chemistry [12, 13, 14, 15]. More precisely, the topological index $Top(G)$ of the graph is a number with the following characteristics: If a graph $H$ is isomorphic to $G$, then $Top(H) = Top(G)$. The concept of topological index comes from Wiener [16]. When he studied the boiling point of paraffin, he named the index as the path number. Later, the path number was renamed Wiener index.

Carbon nanotubes form an interesting class of non-carbon materials [17]. There are three types of nanotubes, namely chiral, zigzag and armchairs nanotubes [18]. These carbon nanotubes show significant mechanical properties [17]. Experimental studies have shown that they belong to the most rigid and elastic known materials [19]. Diudea [20] was the first chemist to consider the topology of nanostructures.

$HAC_5C_6C_7[p,q]$ [21]shown in Figure 1 is constructed by alternating $C_5$, $C_6$ and $C_7$ carbon cycles. It is tube shaped material but we consider it in the form of sheet shown in Figure 2. The two dimensional lattice of $HAC_5C_6C_7[p,q]$ consists of p rows and q periods. Here p denotes the number of pentagons in one row and q is the number of periods in whole lattice. A period consist of three rows (See references [22, 23]). Figures are taken from [24]. Figure 3 is 2D graph of $HAC_5C_6C_7[p,q]$ and figure 4 is line graph of $HAC_5C_6C_7[p,q]$ .

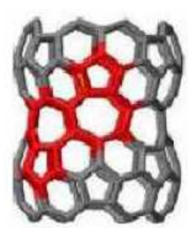

Figure 1. $HAC_5C_6C_7[p,q]$ Nanotube

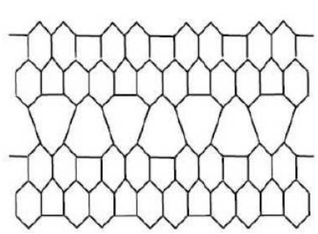

Figure 2. 2D graph of $HAC_5C_6C_7[p,q]$

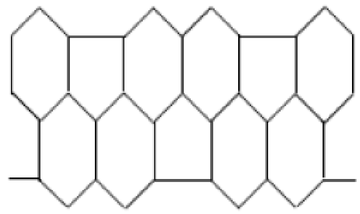

Figure 3. $HAC_5C_6C_7$

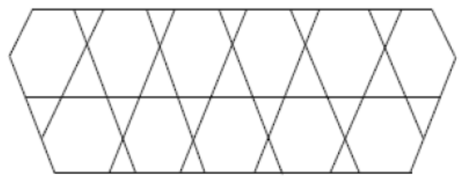

Figure 4. $L(HAC_5C_6C_7)$

The aim of this paper is to compute M-polynomial of the line graph of $HAC_5C_6C_7[p,q]$-nanotube. We also recover many degree-based topological indices of the line graph of $HAC_5C_6C_7[p,q]$ nanotube from this M-polynomial. A line graph has many useful applications in physical chemistry [25, 26] and is defined as: the line graph $L(G)$ of a graph $G$ is the graph each of whose vertex represents an edge of $G$ and two of its vertices are adjacent if their corresponding edges are adjacent in $G$.

## 2. Basic definitions and Literature Review

Throughout this article, we take $G$ as a connected graph. $V(G)$ is the vertex set and $E(G)$ is the edge set. The degree of a vertex $v$ is denoted by

**Definition 2.1.** [27] The M-polynomial of $G$ is defined as:

$$M(G,x,y) = \sum_{\delta \leq i \leq j \leq \triangle} m_{ij}(G) x^i y^j$$

where $\delta = \min\{d_v : v \in V(G)\}$, $\triangle = \max\{d_v : v \in V(G)\}$ and $m_{ij}(G)$ is the edge $uv \in E(G)$ such that $d_u = i$ and $d_v = j$.

Wiener index and its various applications are discussed in [28, 29, 30]. Randić index, $R_{-\frac{1}{2}}(G)$, is introduced by Milan Randić in 1975 defined as: $R_{-\frac{1}{2}}(G) = \sum\limits_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$. For general details about $R_{-\frac{1}{2}}(G)$, and its generalized Randic index, $R_\alpha(G) = \sum\limits_{uv \in E(G)} \frac{1}{(d_u d_v)^\alpha}$ please see [31, 32, 33, 34, 35]. The inverse Randić index is defined as $RR_\alpha(G) = \sum\limits_{uv \in E(G)} (d_u d_v)^\alpha$ Clearly $R_{-\frac{1}{2}}(G)$ is a special case of $R_\alpha(G)$ when $\alpha = \frac{1}{2}$. This index has many applications in diverse areas. Many papers and books such as [36, 37, 38] are written on this topological index as well. Gutman and Trinajstić introduced two indices defined as: $M_1(G) = \sum_{u \in V(G)} (d_u + d_v)$ and $M_2(G) = \sum_{uv \in E(G)} d_u \times d_u$. The second modified Zagreb index is defined as: ${}^m M_2(G) = \sum_{uv \in E(G)} \frac{1}{d_u \times d_u}$. We refer [39, 40, 41, 42, 43] to the readers for comprehensive details of these indices. Other famous indices are Symmetric division index: $SDD(G) = \sum_{uv \in E(G)} \left\{ \frac{\min(d_u,d_v)}{\max(d_u,d_v)}, \frac{\max(d_u,d_v)}{\min(d_u,d_v)} \right\}$ harmonic index: $H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$ inverse sum index:$I(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}$ and augmented Zagreb index: $A(G) = \sum_{uv \in E(G)} \left\{ \frac{\max(d_u,d_v)}{\max(d_u,d_v)} \right\}^3$ [39, 40, 41]. Tables presented in [44, 45, 46, 47, 48] relates some of these well-known degree-based topological indices with M-polynomial with following reserved notations Where $D_x f = x\frac{\partial(f(x,y))}{\partial x}, D_y f = y\frac{\partial(f(x,y))}{\partial y}, S_x = \int_0^x \frac{f(y,t)}{t} dt,\ S_y = \int_0^y \frac{f(x,t)}{t} dt,$ $j(f(x,y)) = f(x,x), Q_\alpha(f(x,y)) = x^\alpha f(x,y)$, for non zero $\alpha$, $j(f(x,y)) = f(x,x)$

## 3. computational Results

In this section, we give our computational results.

**Theorem 3.1.** *Let $G$ be the line graph of $HAC_5C_6C_7[p,q]$ nanotube. Then the M-Polynomial of $G$ is*

$$M(G,x,y) = 2x^2y^2 + 12x^2y^3 + (16p+1)x^3y^3 + (12p+10)x^3y^4 + (70p-37)x^4y^4 \quad (1)$$

*Proof.* Let $G$ be the line graph of $HAC_5C_6C_7[p,q]$ nanotubes where $p$ denotes the number of pentagons in one row and $q$ denotes the number of periods in whole lattice . The edge set of line graph of $HAC_5C_6C_7[p,q]$ with $p \geq 1$ and $q = 2$ has following five partitions,
$E_{2,2} = \{e = vu \in E(HAC_5C_6C_7[p,q]) | d_u = 2, d_v = 2\}$
$E_{2,3} = \{e = vu \in E(HAC_5C_6C_7[p,q]) | d_u = 2, d_v = 3\}$
$E_{3,3} = \{e = vu \in E(HAC_5C_6C_7[p,q]) | d_u = 3, d_v = 3\}$
$E_{3,4} = \{e = vu \in E(HAC_5C_6C_7[p,q]) | d_u = 3, d_v = 4\}$
and
$E_{4,4} = \{e = vu \in E(HAC_5C_6C_7[p,q]) | d_u = 4, d_v = 4\}$.
Now,

$$|E_{2,2}| = 2$$

$$|E_{2,2}| = 12$$

$$|E_{2,2}| = 6p + 1$$

$$|E_{2,2}| = 12p + 10$$

and

$$|E_{2,2}| = 70p - 37$$

So, The M-polynomial of $(HAC_5C_6C_7[p,q])$ is equal to:

$$\begin{aligned}
M(G,x,y) &= \sum_{i\leq j} m_{ij}(G)x^iy^j \\
&= \sum_{2\leq 2} m_{2,2}(G)x^2y^2 + \sum_{2\leq 3} m_{2,3}(G)x^2y^3 \\
&\quad + \sum_{3\leq 3} m_{3,3}(G)x^3y^3 + \sum_{3\leq 4} m_{3,4}(G)x^3y^4 \\
&\quad + \sum_{4\leq 4} m_{4,4}(G)x^4y^4 \\
&= \sum_{E_{2,2}} m_{2,2}(G)x^2y^2 + \sum_{E_{2,3}} m_{2,3}(G)x^2y^3 \\
&\quad + \sum_{E_{3,3}} m_{3,3}(G)x^3y^3 + \sum_{E_{3,4}} m_{3,4}(G)x^3y^4 \\
&\quad + \sum_{E_{4,4}} m_{4,4}(G)x^4y^4 \\
&= |E_{2,2}|x^2y^2 + |E_{2,3}|x^2y^3 + |E_{3,3}|x^3y^3 + |E_{3,4}|x^3y^4 \\
&\quad + |E_{4,4}|x^4y^4 \\
&= 2x^2y^2 + 12x^2y^3 + (16p+1)x^3y^3 + (12p+10)x^3y^4 \\
&\quad + (70p-37)x^4y^4.
\end{aligned}$$

□

**Proposition 3.2.** *Let $G$ be the line graph of $(HAC_5C_6C_7[p,q])$ nanotube, then*

(1) $M_1(G) = 2(85p-19)$
(2) $M_2(G) = 1318p - 383$
(3) ${}^mM_2(G) = \frac{145}{24}p + \frac{163}{144}$
(4) $R_\alpha(G) = (2.3^{2\alpha+1} + 2^{2(\alpha+1)}.3^{\alpha+1} + 35.2^{4\alpha+1})p + (2^{2\alpha+1} + 2^{\alpha+2}3^{\alpha+1}$
$(3^{2\alpha} + 2^{2\alpha+1}.3^{\alpha}.5 - 37.2^{4\alpha})$
(5) $RR_\alpha(G) = \left(\frac{2}{3^{2\alpha-1}} + \frac{1}{2^{2(\alpha-1)}.3^{\alpha-1}} + \frac{35}{2^{4\alpha+1}}\right)p + \left(\frac{1}{2^{2\alpha-1}} + \frac{1}{2^{\alpha-2}3^{\alpha-1}}\right.$
$\left.\frac{1}{3^{2\alpha}} + \frac{5}{2^{2\alpha-1}.3^{\alpha}} - \frac{37}{2^{4\alpha}}\right)$
(6) $SSD(G) = 177p + \frac{127}{6}$.
(7) $H(G) = \frac{321}{14}p + \frac{109}{420}$
(8) $I(G) = \frac{1187}{7}p + \frac{2727}{70}$
(9) $A(G) = \frac{168657029}{108000}p - \frac{19007957}{43200}$

*Proof.* Let

$$M(G,x,y) = 2x^2y^2 + 12x^2y^3 + (16p+1)x^3y^3 + (12p+10)x^3y^4 + (70p-37)x^4y^4$$

Then,

$$D_xf(x,y) = 4x^2y^2 + 24x^2y^3 + 3(16p+1)x^3y^3 + 3(12p+10)x^3y^4 + 4(70p-37)x^4y^4.$$

$D_y f(x,y) = 4x^2y^2+36x^2y^3+3(16p+1)x^3y^3+4(12p+10)x^3y^4+4(70p-37)x^4y^4.$

$D_yD_x f(x,y) = 8x^2y^2+72x^2y^3+9(6p+1)x^3y^3+12(12p+10)x^3y^4+16(70p-37)x^4y^4.$

$S_xS_y f(x,y) = \frac{1}{2}x^2y^2+2x^2y^3+\frac{1}{9}(16p+1)x^3y^3+\frac{1}{12}(12p+10)x^3y^4+\frac{1}{16}(70p-37)x^4y^4.$

$$D_x^\alpha D_y^\alpha f(x,y) = 2^{2\alpha+1}x^2y^2 + 2^{\alpha+2}3^{\alpha+1}x^2y^3 + 3^{2\alpha}(16p+1)x^3y^3 + 3^\alpha 4^\alpha(12p+10)x^3y^3 + 4^{2\alpha}(70p-37)x^3y^3.$$

$$S_x^\alpha S_y^\alpha f(x,y) = \frac{1}{2^{2\alpha-1}}x^2y^2 + \frac{1}{2^{\alpha-2}3^{\alpha-1}}x^2y^3 + \frac{1}{3^{2\alpha}}(16p+1)x^3y^3 + \frac{1}{3^\alpha 4^\alpha}(12p+10)x^3y^4 + \frac{1}{4^{2\alpha}}(70p-37)x^4y^4.$$

$S_yD_x f(x,y) = 2x^2y^2+8x^2y^3+(16p+1)x^3y^3+\frac{3}{4}(12p+10)x^3y^3+(70p-37)x^4y^4.$

$S_xD_y f(x,y) = 2x^2y^2+18x^2y^3+(16p+1)x^3y^3+\frac{3}{4}(12p+10)x^3y^3+(70p-37)x^4y^4.$

$$S_xJf(x,y) = \frac{1}{2}x^4 + \frac{12}{5}x^5 + \frac{9}{6}(6p+1)x^6 + \frac{12}{7}(12P+10)x^7 + 2(70p-37)x^8.$$

$S_xJD_yD_x f(x,y)f(x,y) = 16x^4+\frac{72}{5}x^5+\frac{9}{6}(6p+1)x^6+\frac{12}{7}(12P+10)x^7+2(70p-37)x^8.$

$$S_x^3Q_{-2}JD_x^3D_y^3 f(x,y) = 16x^2 + 96x^3 + \frac{729}{64}(6p+1)x^4 + \frac{1728}{125}(12P+10)x^5 + \frac{4096}{216}(70p-37)x^6.$$

1. First Zagreb Index

$$M_1(G) = (Dx+Dy)[f(x,y)]_{y=x=1} = 2(85p-19).$$

2. Second Zagreb Index

$$M_2(G) = (Dx\cdot Dy)[f(x,y)]_{y=x=1} = 1318p-383.$$

3. Second Modified Zagreb Index

$$^mM_2(G) = (SxSy)[f(x,y)]_{x=y=1} =^m M_2(G) = \frac{145}{24}p + \frac{163}{144}.$$

4. Randić Index

$$R_\alpha(G) = (D_x^\alpha D_y^\alpha)[f(x,y)]_{y=x=1} = (2.3^{2\alpha+1} + 2^{2(\alpha+1)}.3^{\alpha+1} + 35.2^{4\alpha+1})p + (2^{2\alpha+1} + 2^{\alpha+2}3^{\alpha+1}(3^{2\alpha} + 2^{2\alpha+1}.3^\alpha.5 - 37.2^{4\alpha})$$

5. General Randić Index

$$RR_\alpha(G) = (S_x^\alpha S_y^\alpha)[f(x,y)]_{x=y=1} = \left(\frac{2}{3^{2\alpha-1}} + \frac{1}{2^{2(\alpha-1)}.3^{\alpha-1}} + \frac{35}{2^{4\alpha+1}}\right)p + \Big(\frac{1}{2^{2\alpha-1}} + \frac{1}{2^{\alpha-2}3^{\alpha-1}}\frac{1}{3^{2\alpha}} + \frac{5}{2^{2\alpha-1}.3^\alpha} - \frac{37}{2^{4\alpha}}\Big).$$

6. Symmetric Division Index

$$SSD(G) = (D_xS_y + D_yS_x)[f(x,y)] = 177p - \frac{127}{6}.$$

7. Harmonic Index

$$H(G) = 2S_xJ[f(x,y)]_{y=x=1} = \frac{321}{14}p + \frac{109}{420}.$$

8. Inverse Sum Index

$$I(G) = S_x[J(D_xD_y)][f(x,y)]_{y=x=1} = \frac{1187}{7}p + \frac{2727}{70}.$$

9. Augmented Zagreb Index

$$A(G) = S_x^3Q_{-2}JD_x^3D_y^3[f(x,y)]_{x=y=1} = \frac{168657029}{108000}p - \frac{19007957}{43200}.$$

□

## 4. conclusion

In the present article, we computed closed form of M-polynomial for the line graph of $HAC_5C_6C_7[p,q]$ and then we derived many degree-based topological indices as well. Topological indices thus calculated can help us to understand the physical features, chemical reactivity, and biological activities. In this point of view, a topological index can be regarded as a score function which maps each molecular structure to a real number and is used as descriptors of the molecule under testing. These results can also play a vital part in the determination of the significance of silicon-carbon in electronics and industry. For example Randić index is useful for determining physio-chemical properties of alkanes as noticed by chemist Melan Randić in 1975. He noticed the correlation between the Randic index R and several physico-chemical properties of alkanes like, enthalpies of formation, boiling points, chromatographic retention times, vapor pressure and surface areas.

## Competing Interests

The authors do not have any competing interests in the manuscript.

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