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ZAGREB POLYNOMIALS AND REDEFINED ZAGREB INDICES OF LINE GRAPH OF $HAC_5C_6C_7[p,q]$ NANOTUBE

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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 Zagreb-polynomials of line graph of $HAC_5C_6C_7[p,q]$ and compute some degree-based topological indices from it.

Key words and phrases: Zagreb index; Zagreb polynomial, Chemical graph theory; 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].
Cheminformatics 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 [2-5] 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, Randić 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 [12-15]. 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 this 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 $HAC_5C_6C_7[p,q]$.

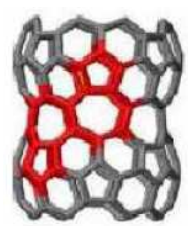

Figure 1. $HAC_5C_6C_7[p,q]$ Nanotube

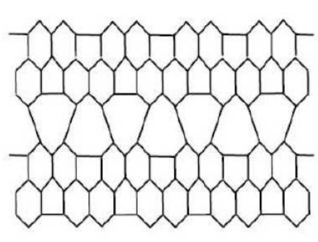

Figure 2. 2D graph of $HAC_5C_6C_7[p,q]$

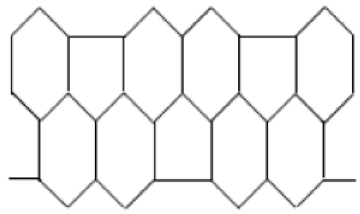

Figure 3. $HAC_5C_6C_7$

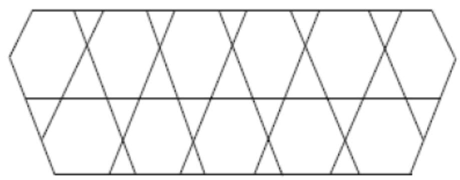

Figure 4. $L(HAC_5C_6C_7)$

The aim of this paper is to compute Zagreb polynomials of the line graph of $HAC_5C_6C_7[p, q]$ nanotube. We also compute some degree-based topological indices of the line graph of $HAC_5C_6C_7[p, q]$ nanotube. 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 d_v, and is equal to number of vertices attached to v.

In the past two decades, a large number of topological indices have been defined and used for correlation analysis in theoretical chemistry, pharmacology, toxicology and environmental chemistry.

The first and second Zagreb indices are one of the oldest and most well-known topological indices defined by Gutman in 1972 and are given different names in the literature, such as the Zagreb group index, Sag. Loeb group parameters and the most common Zagreb index. The Zagreb index is one of the first indices introduced and has been used to study molecular complexity, chirality, ZE isomers and heterogeneous systems. The Zagreb index shows the potential applicability of deriving multiple linear regression models.

The first and the second Zagreb indices [27] are defined as

$$M_1(G) = \prod_{u \in V(G)} (d_u + d_v),$$

$$M_2(G) = \prod_{uv\in E(G)} d_u \times d_u,$$

For details see [28]. Considering the Zagreb indices, Fath-Tabar ([29]) defined first and the second Zagreb polynomials as

$$M_1(G,x) = \sum_{uv\in E(G)} x^{d_u+d_v},$$

and

$$M_2(G,x) = \sum_{uv\in E(G)} x^{d_u.d_v}.$$

The properties of $M_1(G,x)$ and $M_2(G,x)$ for some chemical structures have been studied in the literature [30,31].
After that, in [32], the authors defined the third Zagreb index

$$M_3(G) = \sum_{uv\in E(G)} (d_u - d_v),$$

and the polynomial

$$M_3(G,x) = \sum_{uv\in E(G)} x^{d_u-d_v}.$$

In the year 2016, [33] following Zagreb type polynomials were defined

$$M_4(G,x) = \sum_{uv\in E(G)} x^{d_u(d_u+d_v)},$$

$$M_5(G,x) = \sum_{uv\in E(G)} x^{d_v(d_u+d_v)},$$

$$M_{a,b}(G,x) = \sum_{uv\in E(G)} x^{ad_u+bd_v},$$

$$M'_{a,b}(G,x) = \sum_{uv\in E(G)} x^{(d_u+a)(d_v+b)}.$$

Ranjini *et al.* [34] redefined the Zagreb index, i.e, the redefined first, second and third Zagreb indices of graph G. These indicators appear as

$$ReZG_1(G) = \sum_{uv\in E(G)} \frac{d_u+d_v}{d_u d_v},$$

$$ReZG_2(G) = \sum_{uv\in E(G)} \frac{d_u.d_v}{d_u+d_v},$$

and

$$ReZG_3(G) = \sum_{uv\in E(G)} (d_u+d_v)(d_u.d_v).$$

For details about topological indices and its applications we refer [35-44].

3. Main Results

In this section, we present our computational results.

Theorem 3.1. *Let G be the line graph of $HAC_5C_6C_7$ nanotube. Then*

(1) $M_3(G,x) = 2(38p-17) + 2(6p+11)x$,
(2) $M_4(G,x) = 2x^8 + 12x^{12} + (6p+1)x^{18} + (12p+10)x^{21} + (70p-37)x^{32}$,
(3) $M_5(G,x) = 2x^8 + 12x^{15} + (6p+1)x^{18} + (12p+10)x^{28} + (70p-37)x^{32}$,
(4) $M_{a,b}(G,x) = 2x^{2(a+b)} + 12x^{2a+3b} + (6p+1)x^{3(a+b)} + (12p+10)x^{3a+4b} + (70p-37)x^{4(a+b)}$,
(5) $M'_{a,b}(G,x) = 2x^{(a+2)(b+2)} + 12x^{(a+2)(b+3)} + (6p+1)x^{(a+3)(b+3)} + (12p+10)x^{(a+3)(b+4)} + (70p-37)x^{(a+4)(b+4)}$.

Proof. Let G be the line graph of $HAC_5C_6C_7[p,q]$ nanotube 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,

$$E_1 = E_{2,2} = \{e = uv \in E(HAC_5C_6C_7[p,q]) : d_u = 2, d_v = 2\},$$
$$E_2 = E_{2,3} = \{e = uv \in E(HAC_5C_6C_7[p,q]) : d_u = 2, d_v = 3\},$$
$$E_3 = E_{3,3} = \{e = uv \in E(HAC_5C_6C_7[p,q]) : d_u = 3, d_v = 3\},$$
$$E_4 = E_{3,4} = \{e = uv \in E(HAC_5C_6C_7[p,q]) : d_u = 3, d_v = 4\},$$

and

$$E_5 = E_{4,4} = \{e = uv \in E(HAC_5C_6C_7[p,q]) : d_u = 4, d_v = 4\}.$$

Such that

$$| E_1(G) |= 2,$$
$$| E_2(G) |= 12,$$
$$| E_3(G) |= 6p+1,$$
$$| E_4(G) |= 12p+10,$$
$$| E_5(G) |= 70p+37.$$

(1)

$$\begin{aligned}
M_3(G,x) &= \sum_{uv\in E(G)} x^{d_u-d_v} \\
&= \sum_{uv\in E_1(G)} x^{2-2} + \sum_{uv\in E_2(G)} x^{3-2} + \sum_{uv\in E_3(G)} x^{3-3} + \sum_{uv\in E_4(G)} x^{4-3} \\
&\quad + \sum_{uv\in E_5(G)} x^{4-4} \\
&= | E_1(G) | + | E_2(G) | x + | E_3(G) | + | E_4(G) | x + | E_5(G) | \\
&= 2 + 12x + (6p+1) + (12p+10)x + (70p-37) \\
&= 2(38p-17) + 2(6p+11)x.
\end{aligned}$$

(2)

$$\begin{aligned}
M_4(G,x) &= \sum_{uv\in E(G)} x^{d_u(d_u+d_v)} \\
&= \sum_{uv\in E_1(G)} x^{2(2+2)} + \sum_{uv\in E_2(G)} x^{2(2+3)} + \sum_{uv\in E_3(G)} x^{3(3+3)} \\
&\quad + \sum_{uv\in E_4(G)} x^{3(3+4)} + \sum_{uv\in E_5(G)} x^{4(4+4)} \\
&= \mid E_1(G) \mid x^{8} + \mid E_2(G) \mid x^{10} + \mid E_3(G) \mid x^{18} + \mid E_4(G) \mid x^{28} \\
&\quad + \mid E_5(G) \mid x^{32} \\
&= 2x^8 + 12x^{12} + (6p+1)x^{18} + (12p+10)x^{21} + (70p-37)x^{32}.
\end{aligned}$$

(3)

$$\begin{aligned}
M_5(G,x) &= \sum_{uv\in E(G)} x^{d_v(d_u+d_v)} \\
&= \sum_{uv\in E_1(G)} x^{2(2+2)} + \sum_{uv\in E_2(G)} x^{3(3+2)} + \sum_{uv\in E_3(G)} x^{3(3+3)} \\
&\quad + \sum_{uv\in E_4(G)} x^{4(4+3)} + \sum_{uv\in E_5(G)} x^{4(4+4)} \\
&= \mid E_1(G) \mid x^{8} + \mid E_2(G) \mid x^{15} + \mid E_3(G) \mid x^{18} + \mid E_4(G) \mid x^{28} \\
&\quad + \mid E_5(G) \mid x^{32} \\
&= 2x^8 + 12x^{15} + (6p+1)x^{18} + (12p+10)x^{28} + (70p-37)x^{32}.
\end{aligned}$$

(4)

$$\begin{aligned}
M_{a,b}(G,x) &= \sum_{uv\in E(G)} x^{ad_u+bd_v} \\
&= \sum_{uv\in E_1(G)} x^{2a+2b} + \sum_{uv\in E_2(G)} x^{2a+3b} + \sum_{uv\in E_3(G)} x^{3a+3b} \\
&\quad + \sum_{uv\in E_4(G)} x^{3a+4b} + \sum_{uv\in E_5(G)} x^{4a+4b} \\
&= \mid E_1(G) \mid x^{2(a+b)} + \mid E_2(G) \mid x^{2a+3b} + \mid E_3(G) \mid^{3(a+b)} \\
&\quad + \mid E_4(G) \mid x^{3a+4b} + \mid E_5(G) \mid x^{4(a+b)} \\
&= 2x^{2(a+b)} + 12x^{2a+3b} + (6p+1)x^{3(a+b)} + (12p+10)x^{3a+4b} \\
&\quad +(70p-37)x^{4(a+b)}.
\end{aligned}$$

(5)

$$M'_{a,b}(G,x) = \sum_{uv\in E(G)} x^{(d_u+a)(d_v+b)}$$

$$\begin{aligned}
&= \mid E_1(G) \mid x^{(a+2)(b+2)} + \mid E_2(G) \mid x^{(a+2)(b+3)} \\
&\quad + \mid E_3(G) \mid x^{(a+3)(b+3)} + \mid E_4(G) \mid x^{(a+3)(b+4)} \\
&\quad + \mid E_5(G) \mid x^{(a+4)(b+4)} \\
&= 2x^{(a+2)(b+2)} + 12x^{(a+2)(b+3)} + (6p+1)x^{(a+3)(b+3)} \\
&\quad +(12p+10)x^{(a+3)(b+4)} + (70p-37)x^{(a+4)(b+4)}.
\end{aligned}$$

□

Theorem 3.2. *For every $p \geq 1$ and $q = 2$ consider G be the the graph of $HAC_5C_6C_7[p,q]$ nanotube. Then*
(1) $ReZG_1(G) = 46p$,
(2) $ReZG_1(G) = \frac{1187}{7}p + \frac{2727}{70}$,
(3) $ReZG_1(G) = 2(5146p - 1725)$.

Proof. From the edge partition of line graph of $HAC_5C_6C_7[p,q]$ nanotube given in Theorem 3.1, we have

(1)

$$\begin{aligned}
ReZG_1(G) &= \sum_{uv\in E(G)} \frac{d_u + d_v}{d_u d_v} \\
&= \sum_{uv\in E_1(G)} \frac{d_u + d_v}{d_u d_v} + \sum_{uv\in E_2(G)} \frac{d_u + d_v}{d_u d_v} + \sum_{uv\in E_3(G)} \frac{d_u + d_v}{d_u d_v} \\
&\quad + \sum_{uv\in E_4(G)} \frac{d_u + d_v}{d_u d_v} + \sum_{uv\in E_5(G)} \frac{d_u + d_v}{d_u d_v} \\
&= \mid E_1(G) \mid + \mid E_2(G) \mid \frac{5}{6} + \mid E_3(G) \mid \frac{6}{9} + \mid E_4(G) \mid \frac{7}{12} \\
&\quad + \mid E_5(G) \mid \frac{8}{16} \\
&= 2 + (12)\frac{5}{6} + (6p+1)\frac{6}{9} + (12p+10)\frac{7}{12} + (70p+37)\frac{8}{16} \\
&= 46p.
\end{aligned}$$

(2)

$$\begin{aligned}
ReZG_2(G) &= \sum_{uv\in E(G)} \frac{d_u.d_v}{d_u + d_v} \\
&= \sum_{uv\in E_1(G)} \frac{d_u.d_v}{d_u + d_v} + \sum_{uv\in E_2(G)} \frac{d_u.d_v}{d_u + d_v} + \sum_{uv\in E_3(G)} \frac{d_u.d_v}{d_u + d_v} \\
&\quad + \sum_{uv\in E_4(G)} \frac{d_u.d_v}{d_u + d_v} + \sum_{uv\in E_5(G)} \frac{d_u.d_v}{d_u + d_v} \\
&= \mid E_1(G) \mid + \mid E_2(G) \mid \frac{6}{5} + \mid E_3(G) \mid \frac{9}{6} + \mid E_4(G) \mid \frac{12}{7}
\end{aligned}$$

$$
\begin{aligned}
& + \mid E_5(G) \mid \frac{16}{8} \\
= \;& 2 + (12)\frac{6}{5} + (6p+1)\frac{9}{6} + (12p+10)\frac{12}{7} + (70p+37)\frac{16}{8} \\
= \;& \frac{1187}{7}p + \frac{2727}{70}.
\end{aligned}
$$

(3)

$$
\begin{aligned}
ReZG_2(G) &= \sum_{uv\in E(G)} (d_u.d_v)(d_u+d_v) \\
&= \sum_{uv\in E_1(G)} (d_u.d_v)(d_u+d_v) + \sum_{uv\in E_2(G)} (d_u.d_v)(d_u+d_v) \\
&\quad + \sum_{uv\in E_3(G)} (d_u.d_v)(d_u+d_v) + \sum_{uv\in E_4(G)} (d_u.d_v)(d_u+d_v) \\
&\quad + \sum_{uv\in E_5(G)} (d_u.d_v)(d_u+d_v) \\
&= 16 \mid E_1(G) \mid +30 \mid E_2(G) \mid +54 \mid E_3(G) \mid +84 \mid E_4(G) \mid \\
&\quad +128 \mid E_5(G) \mid \\
&= 32 + 30(12) + 54(6p+1) + 84(12p+10) + 128(70p+37) \\
&= 2(5146p - 1725).
\end{aligned}
$$

□

Competing Interests

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

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