

The second Hyper-Zagreb index of $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotubes

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Abstract

The first and second Hyper-Zagreb indices are the molecular descriptors that describe the structures of chemical compounds and they help us to predict certain physicochemical properties. In this paper, we studied the first and second Hyper-Zagreb indices for certain important chemical structures like line graphs of the $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotubes. Moreover, we defined second Hyper-Zagreb-polynomial of graph G and applied it on the line graphs of the $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotubes. These explicit formulae can

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correlate the chemical structure of molecular graph of nanotube to information about their physical structure.

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1. Introduction

Chemical graph theory which is a fascinating branch of graph theory has many applications related to chemistry. A topological index which is a numerical quantity derived from the chemical graph of a molecule is used to modelling chemical and physical properties of molecules in QSPR/QSAR researches [6]. Topological indices are the molecular descriptors that describe the structures of chemical compounds and they help us to predict certain physicochemical properties[2, 3]. Rao Li et al. [25] by using first Zagreb index of a graph, presented sufficient conditions for some Hamiltonian properties of the line graph of a graph. Wei Gao et al. [26] studied the Hyper-Zagreb index for an infinite family of nanostar dendrimer. In (2019) Mahdiah Azari [27] computed the multiplicative sum Zagreb index of some chemical graphs such as polyphenylene chains and spiro chains and in (2021) Alsharafi et al. [28] investigated the F-index and coindex of V-Phenylenic Nanotubes and Nanotorus and their molecular complement graphs. Ayache et al. [29] studied the Second Hyper-Zagreb Coindex of chemical graphs and some applications. Here we continue this line of research by exploring the behavior of the second Hyper-Zagreb index for certain important chemical structures like line graphs of the $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotubes. The first and second Zagreb indices can be regarded as one of the oldest graph invariants which was defined in (1972) by Gutman and Trinajstić. The first and second Zagreb indices defined for a molecular graph G as:

$$M_1(G) = \sum_{uv \in E(G)} [\delta_G(u) + \delta_G(v)], \quad M_2(G) = \sum_{uv \in E(G)} \delta_G(u)\delta_G(v),$$

The first and second Zagreb coindices have been introduced by A.R. Ashrafi, T. Došlić, and A. Hamzeh in 2010 [6]. They are respectively defined as:

$$\overline{M}_1(G) = \sum_{uv \notin E(G)} [\delta_G(u) + \delta_G(v)], \quad \overline{M}_2(G) = \sum_{uv \notin E(G)} \delta_G(u)\delta_G(v),$$

Furtula and Gutman in 2015 introduced forgotten index (F-index) [7] which is defined as:

$$F(G) = \sum_{v \in V(G)} \delta_G^3(v) = \sum_{uv \in E(G)} (\delta_G^2(u) + \delta_G^2(v))$$

Furtula et al. in (2015) defined forgotten coindex (F-coindex) [8] as the following:

$$\bar{F}(G) = \sum_{uv \notin E(G)} (\delta_G^2(u) + \delta_G^2(v))$$

A. Alameri et al. [9], [10]. in 2020 defined the (Y-index) and (Y-coindex), which are defined respectively such as:

$$Y(G) = \sum_{uv \in E(G)} [\delta_G^3(u) + \delta_G^3(v)], \quad \bar{Y}(G) = \sum_{uv \notin E(G)} [\delta_G^3(u) + \delta_G^3(v)]$$

In 2013, G.H. Shirdel, H. Rezapour and A.M. Sayadi [22] introduced degree-based of Zagreb indices named Hyper-Zagreb index which is defined as:

$$HM(G) = \sum_{uv \in E(G)} (\delta_G(u) + \delta_G(v))^2$$

In 2016, Maryam Veylaki et al. [23] introduced degree-based of Zagreb indices named Hyper-Zagreb coindex which is defined as:

$$\overline{HM}(G) = \sum_{uv \notin E(G)} (\delta_G(u) + \delta_G(v))^2$$

In 2016, Wei Gao et al. [24]. defined second Hyper-Zagreb index of a graph G , which is defined as :

$$HM_2(G) = \sum_{uv \in E(G)} (\delta_G(u)\delta_G(v))^2$$

Then, Farahani et al [1]. computed the first and second Zagreb polynomials of $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ and their indices, B. Zhao et al. [12]. computed the Redefined Zagreb indices of $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$. F. Deng et al. [13]. studied the topological Indices of the Pent-Heptagonal Nanosheets VC_5C_7 and HC_5C_7 , and there are a lot of researchers who have studied some topological Indices on VC_5C_7 and HC_5C_7 nanotubes that cannot be all mentioned here. In this study, we compute the first and second Hyper-Zagreb indices for certain important chemical structures like line graphs of the $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotubes. G.H. Shirdel et al. [22] in (2013) and Alsharafi et al. [16] in (2020) computed the Hyper-Zagreb index of some special graph and graph

operation. A. Modabish et al. [21], in 2021 studied the second Hyper-Zagreb index of some special graph and graph operations. Nanotubes play an important role in many applications such as Energy storage, Bioelectronics and Optoelectronics [19]. Because of the unique structural, electrical, optical, and mechanical properties, graphene nanosheets drew dramatic attention of academic and industrial research [13, 20] and as nanotubes introduced into graphene could be extremely useful and exploited to generate novel, innovative, and useful materials and devices. So, the property of VC_5C_7 and HC_5C_7 nanostructures has become an active area of research [13]. Here we present the HM – index and HM_2 – index and their topological polynomials of $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotubes which are useful for surveying structure of nanotubes. Any unexplained terminology is standard, typically as in [11, 14, 15, 16, 17, 18].

2. Main results

In this section, we compute the first and second Hyper-Zagreb indices for certain important chemical structures like line graphs of the $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotubes. Moreover, we define HM_2 – polynomial of graph G and apply it on the line graphs of the $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotubes.

Theorem 2.2 : [1] *The first and second Zagreb indices of $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotube (Figure 1) and (Figure 2) respectively, are given by*

$$M_1(VC_5C_7[p, q]) = 12p[12q + 2],$$

$$M_2(VC_5C_7[p, q]) = p[216q + 18],$$

$$M_1(HC_5C_7[p, q]) = p[72q + 20],$$

$$M_2(HC_5C_7[p, q]) = p[108q + 16].$$

2.1 Second Hyper-Zagreb index of $VC_5C_7[p, q]$ nanotube ($p, q \geq 1$)

Theorem 2.1.1 : *The HM_2 – index of $VC_5C_7[p, q]$ nanotube (Figure 1) is given by*

$$HM_2(VC_5C_7[p, q]) = p[1944q - 54].$$

Proof: By definition of the HM_2 – index $HM_2(G) = \sum_{uv \in E(G)} [\delta_G(u)\delta_G(v)]^2$, and by replacing each G with $VC_5C_7[p, q]$, which yield to $HM_2(VC_5C_7[p, q])$

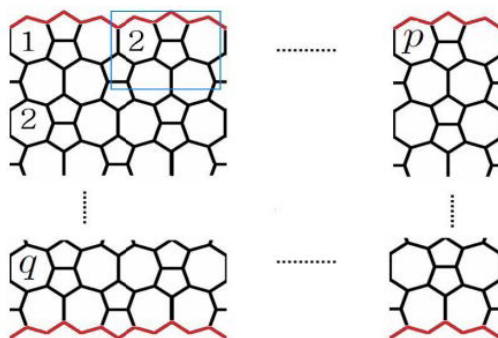


Figure 1

Molecular graph of a $VC_5C_7[p, q]$ nanotube.

Table 1

The edge partition of $VC_5C_7[p, q]$ nanotubes.

Edge partition	$E_5 = E_6^*$	$E_6 = E_9^*$
Cardinality	$12p$	$24pq - 6p$

Table 2

The vertex partition of $VC_5C_7[p, q]$ nanotubes.

Vertex partition	V_2	V_3
Cardinality	$3p + 3p$	$16pq$

$= \sum_{uv \in E(VC_5C_7[p, q])} [\delta_{VC_5C_7[p, q]}(u) \delta_{VC_5C_7[p, q]}(v)]^2$, and the partitions of the vertex set and edge set $V(VC_5C_7[p, q]), E(VC_5C_7[p, q])$, of $VC_5C_7[p, q]$ nanotube are given in (Tables 1, 2) respectively [1].

The edge set of $VC_5C_7[p, q]$ is divided into three edge partitions based on the sum of degrees of the end vertices as:

$$E_5(VC_5C_7[p, q]) = E_6^* = \{e = uv \in E(VC_5C_7[p, q]) : \delta(u) = 2, \delta(v) = 3\},$$

$$E_6(VC_5C_7[p, q]) = E_9^* = \{e = uv \in E(VC_5C_7[p, q]) : \delta(u) = 3, \delta(v) = 3\},$$

Thus:

$$HM_2(VC_5C_7[p, q]) = \sum_{uv \in E(VC_5C_7[p, q])} [\delta_{VC_5C_7[p, q]}(u) \delta_{VC_5C_7[p, q]}(v)]^2$$

$$\begin{aligned}
&= \sum_{uv \in E_6^+(VC_5C_7[p,q])} [\delta_{VC_5C_7[p,q]}(u)\delta_{VC_5C_7[p,q]}(v)]^2 \\
&+ \sum_{uv \in E_9^+(VC_5C_7[p,q])} [\delta_{VC_5C_7[p,q]}(u)\delta_{VC_5C_7[p,q]}(v)]^2 \\
&= 36 |E_6^+(VC_5C_7[p,q])| + 81 |E_9^+(VC_5C_7[p,q])| \\
&= 36 |E_6^+(VC_5C_7[p,q])| + 81 |E_9^+(VC_5C_7[p,q])| \\
&= 432p + 81[24pq - 6p] \\
&= 1944pq - 54p.
\end{aligned}$$

Definition 2.1.2 : The HM_2 – *polynomial* of graph G defined as:

$$HM_2(G, x) = \sum_{uv \in E(G)} x^{[\delta_G(u)\delta_G(v)]^2}$$

Theorem 2.1.3 : The HM_2 – *polynomial* of $VC_5C_7[p, q]$ nanotube (Figure 1) is given by

$$HM_2(VC_5C_7[p, q], x) = 6p[2x^{36} + [4q - 1]x^{81}].$$

Proof: By definition of the HM_2 – *polynomial* of graph G (2.1.2) and as (Theorem 2.1.1) the partitions of the vertex set and edge set $V(VC_5C_7[p, q]), E(VC_5C_7[p, q])$, of $VC_5C_7[p, q]$ nanotube are given in (Tables 1, 2) respectively we have,

$$\begin{aligned}
HM_2(VC_5C_7[p, q], x) &= \sum_{uv \in E(VC_5C_7[p, q])} x^{[\delta_{VC_5C_7[p, q]}(u)\delta_{VC_5C_7[p, q]}(v)]^2} \\
&= \sum_{uv \in E_6^+(VC_5C_7[p, q])} x^{[\delta_{VC_5C_7[p, q]}(u)\delta_{VC_5C_7[p, q]}(v)]^2} \\
&+ \sum_{uv \in E_9^+(VC_5C_7[p, q])} x^{[\delta_{VC_5C_7[p, q]}(u)\delta_{VC_5C_7[p, q]}(v)]^2} \\
&= |E_6^+(VC_5C_7[p, q])| x^{36} + |E_9^+(VC_5C_7[p, q])| x^{81} \\
&= 12px^{36} + [24pq - 6p]x^{81} \\
&= 6p[2x^{36} + [4q - 1]x^{81}].
\end{aligned}$$

We can also get the HM_2 – *index* of $VC_5C_7[p, q]$ nanotube by derivating the relation HM_2 – *polynomial* of $VC_5C_7[p, q]$ nanotube above as:

$$\begin{aligned} HM_2(VC_5C_7[p, q]) &= \frac{\partial Y(VC_5C_7[p, q], x)}{\partial x} \Big|_{x=1} = \frac{\partial [12px^{36} + 6p[4q-1]x^{81}]}{\partial x} \Big|_{x=1} \\ &= 1944pq - 54p. \end{aligned}$$

Theorem 2.1.4 : *The F – index of $VC_5C_7[p, q]$ nanotube (Figure 1) is given by*

$$F(VC_5C_7[p, q]) = 48p[1 + 9q].$$

Proof: By definition of forgotten index (F-index) and Theorem (2.1.1). Then,

$$\begin{aligned} F(VC_5C_7[p, q]) &= \sum_{uv \in E(VC_5C_7[p, q])} [\delta_{VC_5C_7[p, q]}^2(u) + \delta_{VC_5C_7[p, q]}^2(v)] \\ &= \sum_{uv \in E_6^*(VC_5C_7[p, q])} [\delta_{VC_5C_7[p, q]}^2(u) + \delta_{VC_5C_7[p, q]}^2(v)] \\ &\quad + \sum_{uv \in E_9^*(VC_5C_7[p, q])} [\delta_{VC_5C_7[p, q]}^2(u) + \delta_{VC_5C_7[p, q]}^2(v)] \\ &= 13 |E_6^*(VC_5C_7[p, q])| + 18 |E_9^*(VC_5C_7[p, q])| \\ &= 156p + 18[24pq - 6p] \\ &= 48p[1 + 9q]. \end{aligned}$$

□

Theorem 2.1.5: *The HM – index of $VC_5C_7[p, q]$ nanotube (Figure 1) is given by*

$$HM(VC_5C_7[p, q]) = p[864q + 84].$$

Proof: By definition of Hyper-Zagreb index (HM-index) and Theorem (2.1.1). Then,

$$\begin{aligned} HM(VC_5C_7[p, q]) &= \sum_{uv \in E(VC_5C_7[p, q])} [\delta_{VC_5C_7[p, q]}(u) + \delta_{VC_5C_7[p, q]}(v)]^2 \\ &= \sum_{uv \in E_6^*(VC_5C_7[p, q])} [\delta_{VC_5C_7[p, q]}(u) + \delta_{VC_5C_7[p, q]}(v)]^2 \\ &\quad + \sum_{uv \in E_9^*(VC_5C_7[p, q])} [\delta_{VC_5C_7[p, q]}(u) + \delta_{VC_5C_7[p, q]}(v)]^2 \\ &= 25 |E_6^*(VC_5C_7[p, q])| + 36 |E_9^*(VC_5C_7[p, q])| \\ &= p[864q + 84]. \end{aligned}$$

□

Table 3
Some topological indices values of $H = VC_5C_7[p, q]$ nanotubes.

p	q	$M_1(H)$	$M_2(H)$	$F(H)$	$HM(H)$	$HM_2(H)$
1	1	168	234	480	948	18.900×10^2
1	2	312	450	912	1812	38.340×10^2
1	3	456	666	1344	2676	57.780×10^2
2	1	336	468	960	1896	37.800×10^2
2	2	624	900	1824	3624	76.680×10^2
2	3	912	1332	2688	5352	11.556×10^3
3	1	504	702	1440	2844	56.700×10^2
3	2	936	1350	2736	5436	11.502×10^3
3	3	1368	1996	4032	8028	17.334×10^3

In (Table 3) some index values of $VC_5C_7[p, q]$ nanotubes. formulas reported in (Theorem 2.1.1), (Theorem 2.1.4) and (Theorem 2.1.5) for the $VC_5C_7[p, q]$ nanotube. In table it show that values of first and second Zagreb indices, HM_2 – index, F – index and HM – index are in increasing order as the values of p, q increase.

2.2 Second Hyper-Zagreb index of $HC_5C_7[p, q]$ nanotube ($p, q \geq 1$)

Theorem 2.2.1: The HM_2 – index of $HC_5C_7[p, q]$ nanotube (Figure 2) is given by

$$HM_2(HC_5C_7[p, q]) = p[972q - 20]$$

Proof: By definition of the HM_2 – index and by [1] the partitions of the vertex set and edge set $V(HC_5C_7[p, q]), E(HC_5C_7[p, q])$, of $HC_5C_7[p, q]$ nanotubes are given in (Tables 4, 5) respectively.

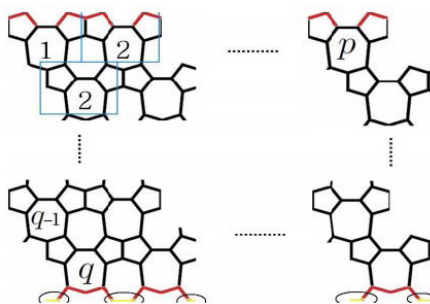


Figure 2
Molecular graph of a $HC_5C_7[p, q]$ nanotube.

Table 4
The edge partition of $HC_5C_7[p, q]$ nanotubes.

Edge partition	$E_4 = E_4^*$	$E_5 = E_6^*$	$E_6 = E_9^*$
Cardinality	p	$8p$	$12pq - 4p$

Table 5
The vertex partition of $HC_5C_7[p, q]$ nanotubes.

Vertex partition	V_2	V_3
Cardinality	$5p$	$8pq$

The edge set of $HC_5C_7[p, q]$ is divided into three edge partitions based on the sum of degrees of the end vertices as:

$$E_4(HC_5C_7[p, q]) = E_4^* = \{e = uv \in E(HC_5C_7[p, q]) : \delta(u) = 2, \delta(v) = 2\},$$

$$E_5(HC_5C_7[p, q]) = E_6^* = \{e = uv \in E(HC_5C_7[p, q]) : \delta(u) = 2, \delta(v) = 3\},$$

$$E_6(HC_5C_7[p, q]) = E_9^* = \{e = uv \in E(HC_5C_7[p, q]) : \delta(u) = 3, \delta(v) = 3\},$$

Thus:

$$\begin{aligned}
 HM_2(HC_5C_7[p, q]) &= \sum_{uv \in E(HC_5C_7[p, q])} [\delta_{HC_5C_7[p, q]}(u) \delta_{HC_5C_7[p, q]}(v)]^2 \\
 &= \sum_{uv \in E_4^*(HC_5C_7[p, q])} [\delta_{HC_5C_7[p, q]}(u) \delta_{HC_5C_7[p, q]}(v)]^2 \\
 &\quad + \sum_{uv \in E_6^*(HC_5C_7[p, q])} [\delta_{HC_5C_7[p, q]}(u) \delta_{HC_5C_7[p, q]}(v)]^2 \\
 &\quad + \sum_{uv \in E_9^*(HC_5C_7[p, q])} [\delta_{HC_5C_7[p, q]}(u) \delta_{HC_5C_7[p, q]}(v)]^2 \\
 &= 16 |E_4^*(HC_5C_7[p, q])| + 36 |E_6^*(HC_5C_7[p, q])| + 81 |E_9^*(HC_5C_7[p, q])| \\
 &= 16p + 288p + 81[12pq - 4p].
 \end{aligned}$$

□

Theorem 2.2.2 : The HM_2 – polynomial of $HC_5C_7[p, q]$ nanotube (Figure 2) is given by

$$HM_2(HC_5C_7[p, q], x) = p[x^{16} + 8x^{36} + [12q - 4]x^{81}].$$

Proof: By definition of the HM_2 – *polynomial* of graph G (2.1.2) and as (Theorem 2.1.1) the partitions of the vertex set and edge set of $(HC_5C_7[p, q])$ nanotubes. Thus,

$$\begin{aligned}
 HM_2(HC_5C_7[p, q], x) &= \sum_{uv \in E(HC_5C_7[p, q])} x^{[\delta_{HC_5C_7[p, q]}(u) \delta_{HC_5C_7[p, q]}(v)]^2} \\
 &= \sum_{uv \in E_4^*(HC_5C_7[p, q])} x^{[\delta_{HC_5C_7[p, q]}(u) \delta_{HC_5C_7[p, q]}(v)]^2} \\
 &\quad + \sum_{uv \in E_6^*(HC_5C_7[p, q])} x^{[\delta_{HC_5C_7[p, q]}(u) \delta_{HC_5C_7[p, q]}(v)]^2} \\
 &\quad + \sum_{uv \in E_9^*(HC_5C_7[p, q])} x^{[\delta_{HC_5C_7[p, q]}(u) \delta_{HC_5C_7[p, q]}(v)]^2} \\
 &= |E_4^*(HC_5C_7[p, q])| x^{16} + |E_6^*(HC_5C_7[p, q])| x^{36} + |E_9^*(HC_5C_7[p, q])| x^{81} \\
 &= px^{16} + 8px^{36} + [12pq - 4p]x^{81} \\
 &= p[x^{16} + 8x^{36} + [12q - 4]x^{81}].
 \end{aligned}$$

□

We can also get the HM_2 – *index* of $HC_5C_7[p, q]$ nanotube by derivating the relation HM_2 – *polynomial* of $HC_5C_7[p, q]$ nanotube above as:

$$\begin{aligned}
 HM_2(HC_5C_7[p, q]) &= \frac{\partial Y(HC_5C_7[p, q], x)}{\partial x} \Big|_{x=1} = \frac{\partial [px^{16} + 8px^{36} + p[12q - 4]x^{81}]}{\partial x} \Big|_{x=1} \\
 &= 972pq - 20p.
 \end{aligned}$$

Theorem 2.2.3 : The F – *index* of $HC_5C_7[p, q]$ nanotube (Figure 2) is given by

$$F(HC_5C_7[p, q]) = p[216q + 40].$$

Proof: By definition of forgotten index (F-index) and as (Theorem 2.2.1) the partitions of the vertex set and edge set $V(HC_5C_7[p, q]), E(HC_5C_7[p, q])$, of $HC_5C_7[p, q]$ nanotubes are given in (Tables 4, 5) respectively. Then,

$$\begin{aligned}
 F(HC_5C_7[p, q]) &= \sum_{uv \in E(HC_5C_7[p, q])} [\delta_{HC_5C_7[p, q]}^2(u) + \delta_{HC_5C_7[p, q]}^2(v)] \\
 &= \sum_{uv \in E_4^*(HC_5C_7[p, q])} [\delta_{HC_5C_7[p, q]}^2(u) + \delta_{HC_5C_7[p, q]}^2(v)] \\
 &\quad + \sum_{uv \in E_6^*(HC_5C_7[p, q])} [\delta_{HC_5C_7[p, q]}^2(u) + \delta_{HC_5C_7[p, q]}^2(v)]
 \end{aligned}$$

$$\begin{aligned}
& + \sum_{uv \in E_9^*(HC_5C_7[p, q])} [\delta_{HC_5C_7[p, q]}^2(u) + \delta_{HC_5C_7[p, q]}^2(v)] \\
& = 8 |E_4^*(HC_5C_7[p, q])| + 13 |E_6^*(HC_5C_7[p, q])| + 18 |E_9^*(HC_5C_7[p, q])| \\
& = 8p + 104p + 18[12pq - 4p].
\end{aligned}$$

□

Theorem 2.2.4: The Hyper-Zagreb index (HM-index) of $HC_5C_7[p, q]$ nanotube (Figure 2) is given by

$$HM(HC_5C_7[p, q]) = p[972q - 108]$$

Proof: By definition of HM – index and as (Theorem 2.2.1) the partitions of the vertex set and edge set $V(HC_5C_7[p, q]), E(HC_5C_7[p, q])$, of $HC_5C_7[p, q]$ nanotubes are given in (Tables 4, 5) respectively. Then,

$$\begin{aligned}
HM(HC_5C_7[p, q]) &= \sum_{uv \in E(HC_5C_7[p, q])} [\delta_{HC_5C_7[p, q]}(u) + \delta_{HC_5C_7[p, q]}(v)]^2 \\
&= \sum_{uv \in E_4^*(HC_5C_7[p, q])} [\delta_{HC_5C_7[p, q]}(u) + \delta_{HC_5C_7[p, q]}(v)]^2 \\
&+ \sum_{uv \in E_6^*(HC_5C_7[p, q])} [\delta_{HC_5C_7[p, q]}(u) + \delta_{HC_5C_7[p, q]}(v)]^2 \\
&+ \sum_{uv \in E_9^*(HC_5C_7[p, q])} [\delta_{HC_5C_7[p, q]}(u) + \delta_{HC_5C_7[p, q]}(v)]^2 \\
&= 16 |E_4^*(HC_5C_7[p, q])| + 25 |E_6^*(HC_5C_7[p, q])| + 81 |E_9^*(HC_5C_7[p, q])| \\
&= 16p + 200p + 81[12pq - 4p].
\end{aligned}$$

□

In (Table 6) some index and coindex values of $HC_5C_7[p, q]$ nanotubes. formulas reported in (Theorem 2.2.1), (Theorem 2.2.3) and (Theorem 2.2.4) for the $HC_5C_7[p, q]$ nanotube. In table it show that values of first and second Zagreb indices, HM_2 – index, F – index and HM – index are in increasing order as the values of p, q increase.

3. Conclusion

The present study has computed the Second Hyper-Zagreb index of line graphs of the $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotubes. The study also

Table 6
Some topological indices values of $G = HC_5C_7[p, q]$ nanotubes.

p	q	$M_1(G)$	$M_2(G)$	$F(G)$	$HM(G)$	$HM_2(G)$
1	1	92	124	256	728	95.200×10^2
1	2	164	232	472	1376	19.240×10^2
1	3	236	340	688	2024	28.960×10^2
2	1	184	248	512	1456	19.040×10^2
2	2	328	464	944	2752	38.480×10^2
2	3	472	680	1376	4048	57.920×10^2
3	1	276	372	768	2184	28.560×10^2
3	2	492	496	1416	4128	57.720×10^2
3	3	708	1020	2064	6072	86.880×10^2

has defined Second Hyper Zagreb-polynomial of graph G and applied it on the line graphs of the $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotubes.

References

- [1] M. R. Farahani , First and Second Zagreb polynomials of $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotubes, *International Letters of Chemistry, Physics and Astronomy*. 12, (2014), 56-62.
- [2] M. Alsharafi, M. Shubatah, A. Alameri, The First and Second Zagreb Index of Complement Graph and Its Applications of Molecular Graph, *Asian Journal of Probability and Statistics*. 8(3), (2020), 15-30.
- [3] M. Alsharafi, M. Shubatah, A. Alameri, On the Hyper-Zagreb coindex of some Graphs, *J. Math. Comput. Sci.* 10(5), (2020), 1875-1890.
- [4] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* 17, (1972), 535-538.
- [5] M. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, The first and second Zagreb indices of some graph operations, *Discrete applied mathematics* 157(4), (2009), 804-811.
- [6] A. Ashrafi, T. Došlić, A. Hamzeh, , The Zagreb coindices of graph operations, *Discret. Appl.Math*, 158, (2010), 1571-1578.
- [7] B. Furtula and I. Gutman., A forgotten topological index, *J. Math. Chem.* 53(4),(2015),1184-1190.

- [8] B. Furtula, I. Gutman, et al., On an old/new degree-based topological index, *Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.)* 40, (2015), 19-31.
- [9] A. Alameri, N. Al-Naggar, M. Al-Rumaima, M. Alsharafi, Y-index of some graph operations, *International Journal of Applied Engineering Research (IJAER)*. 15 (2),(2020), 173-179.
- [10] A. Alameri, M. Al-Rumaima, M. Almazah, Y-coindex of graph operations and its applications of molecular descriptors, *Journal of Molecular Structure*, Volume: 1221, (2020), art. no. 128754.
- [11] M. Alsharafi, M. Shubatah, A. Alameri, The forgotten index of complement graph operations and its applications of molecular graph, *Open Journal of Discrete Applied Mathematics*. 3(3), (2020), 53-61.
- [12] B. Zhao, J. Gan, H. Wu, Redefined Zagreb indices of Some Nano Structures, *Applied Mathematics and Nonlinear Sciences* 1(1), (2016), 291-300.
- [13] F. Deng, X. Zhang, M. Alaeiyan, A. Mehboob, M. Farahani, Topological Indices of the Pent-Heptagonal Nanosheets VC_5C_7 and HC_5C_7 , *Advances in Materials Science and Engineering* Volume 2019, Article ID 9594549, 12 pages.
- [14] A. Alameri, M. Shubatah, M. Alsharafi, Zagreb indices, Hyper Zagreb indices and Redefined Zagreb indices of conical graph, *Advances in Mathematics: Scientific Journal*, 9(6), (2020), 3631-3642.
- [15] J. Bao Liu, M. Younas, M. Habib, M. Yousaf, W. Nazeer, M-Polynomials and Degree-Based Topological Indices of $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ Nanotubes, *Open Access Journal*, 7, (2019), 41125-41132.
- [16] M. Alsharafi, M. Shubatah, On the Hyper-Zagreb index of some Graph Binary Operations, *Asian Research Journal of Mathematics* 16(4) (2020), 12-24.
- [17] M. Alsharafi, M. Shubatah, A. Alameri, The hyper-Zagreb index of some complement graphs, *Advances in Mathematics: Scientific Journal*, 9(6), (2020), 3631-3642.
- [18] A. Modabish, D. Lotfi, M. El Marraki, Formulas for the Number of Spanning Trees in a Maximal Planar Map, *Applied Mathematical Sciences*, 5(64), (2011), 3147-3159.
- [19] B. Furtula, I. Gutman, M. Dehmer, On structure-sensitivity of degree-based topological indices, *Appl. Math. Comput.* 219(17), (2013), 8973-8978.

- [20] Z. Shao, M. K. Siddiqui & M. H. Muhammad, Computing Zagreb Indices and Zagreb Polynomials for Symmetrical Nanotubes, *Symmetry Journal*. 10(7), (2018), art. no. 244.
- [21] A. Modabish, A. Alameri, M. Gumaan, M. Alsharafi, The second hyper-Zagreb index of graph operations, *J. Math. Comput. Sci.* 11(2), (2021), 1455-1469.
- [22] G.H. Shirdel, H. Rezapour and A.M. Sayadi, The hyper-Zagreb index of graph operations, *Iranian J. Math. Chem.* 4 (2), (2013), 213-220.
- [23] M. Veylaki, M.J. Nikmehr and H. A.Tavallaee, The third and hyper-Zagreb coindices of some graph operations, *J. Appl. Math. Comput.* 50, (2016), 315-325.
- [24] Wei Gao, M. R. Farahani, M. K. Siddiqui, On the First and Second Zagreb and First and Second Hyper-Zagreb Indices of Carbon Nanocones $CNC_k[n]$, *Journal of Computational and Theoretical Nanoscience*. 13(10), (2016), 7475-7482.
- [25] Rao Li & Megan M. Taylor, The first zagreb index and some hamiltonian properties of the line graph of a graph, *Journal of Discrete Mathematical Sciences and Cryptography*. 20(2), (2017), 445-451.
- [26] Wei Gao & M. R. Farahani, The Hyper-Zagreb index for an infinite family of nanostar dendrimer, *Journal of Discrete Mathematical Sciences and Cryptography*. 20(2), (2017), 515-523.
- [27] Mahdiah Azari, Multiplicative sum Zagreb index of chain and chain-cycle graphs, *Journal of Information and Optimization Sciences*. 40(7), (2019), 1529-1541.
- [28] M. Alsharafi & A. Alameri, The F-index and coindex of V-Phenylenic Nanotubes and Nanotorus and their molecular complement graphs, *Nanosystems Physics Chemistry Mathematics*. 12(3), (2021), 263-270.
- [29] A. Ayache, A. Alameri, M. Alsharafi, and H. Ahmed, The Second Hyper-Zagreb Coindex of Chemical Graphs and Some Applications, *Journal of Chemistry*. vol. 2021, (2021): Article ID 3687533, 8 pages.

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