TWMS J. App. and Eng. Math. V.14, N.2, 2024, pp. 433-445

THE Y- INDEX AND COINDEX OF $VC_5C_7[p,q]$ AND $HC_5C_7[p,q]$ NANOTUBES

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Abstract. The Y-index and coindex are degree based molecular structure descriptors that have been shown to give a high degree of predictability compare to Zagreb indices and F-index and their coindices for some physicochemical properties of octane isomers. In this paper, we studied the $Y - index$ and $Y - coindex$ for certain important chemical structures like line graphs of the $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$ nanotubes and their molecular complement graph. Moreover, we defined $Y - polynomial$ 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 correlate the chemical structure of molecular graph of nanotube to information about their physical structure.

Keywords: Y-index, Y-coindex, $VC_5C_7[p,q]$ nanotube, $HC_5C_7[p,q]$ nanotube, molecular graph, molecular complement graph.

AMS Subject Classification: 05C12, 05C90, 90C35, 05A15, 05C05, 05C50.

1. Introduction

Chemical graph theory is a mixture of chemistry and mathematics both play an important role in chemical graph theory. Chemistry provides a chemical compound and graph theory transform this chemical compound into a molecular graph which further studied by different aspects such as topological indices[1]. Topological indices are the molecular descriptors that describe the structures of chemical compounds and they help us to predict certain physicochemical properties[2, 3]. In these frameworks, the molecular is represented as a graph in which each atom is expressed as a vertex and covalent bounds between atoms are represented as edges between vertices. Topological indices were introduced to determine the chemical and pharmaceutical properties. The first and second Zagreb indices can

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§ Manuscript received: August 01, 2021; accepted: November 8, 2021.

be regarded as one of the oldest graph invariants which was defined in (1972) by Gutman and Trinajstić [4, 5]. The first and second Zagreb indices defined for a molecular graph G as:

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

The first and second Zagreb coindices have been introduced by Ashrafi et al. [6] in (2010). They are respectively defined as:

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

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

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

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

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

Alameri et al. [9, 10] in (2020) introduced $Y-index$, $Y-coindex$, and defined respectively as follows:

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

In (2005) Li and Zheng [22] introduced the first general Zagreb index as:

$$M_1^\alpha(G) = \sum_{v\in V(G)} {\delta_G}^{\alpha+1}(v) = \sum_{uv\in E(G)} \delta_G^\alpha(u) + \delta_G^\alpha(v).$$

We note that, the first Zagreb index, the F-index and the Y-index are special cases from the first general Zagreb index, when $\alpha = 1, 2, 3$ respectively.

By Li and Gutman, the general Rendić index [23], defined as follows:

$$R^\alpha(G) = \sum_{uv\in E(G)} [\delta_G(u)\,\delta_G(v)]^\alpha.$$

And we see that, the Rendić, the second Zagreb, and the second Hyper-Zagreb indices are special cases from the general Rendić index, when $\alpha = -1/2, 1, 2$ respectively.

The general zeroth-order Randić coindex was defined in [24], as:

$${}^0\overline{R}^\alpha(G) = \sum_{uv\notin E(G)} [\delta_G^\alpha(u) + \delta_G^\alpha(v)].$$

Also, we note that, the first Zagreb coindex, the F-coindex and the Y-coindex are special cases from the general zeroth-order Randić coindex, when $\alpha = 1, 2, 3$ respectively, for more detail, we refer to [24, 25].

Then, Farahani et al. [11] computed the first and second Zagreb polynomials of VC_5C_7 and HC_5C_7 and their indices, B. Zhao et al. [12] computed the Redefined Zagreb indices of $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$. 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 $Y - index$ and $Y - coindex$ of two nanotubes VC_5C_7 and HC_5C_7 and their polynomials. Alameri et al. [9, 10] in (2020) defined the (Y-index) and (Y-coindex) and studied their of some special graph and graph operation. 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, 21]. 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 $Y-index$ and $Y-coindex$ 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 [14, 15, 16, 17, 18].

2. Preliminaries

In this section, we give some basic and preliminary concepts which we shall use later. In this paper, we consider a finite connected graph G that has no loops or multiple edges. The vertex and the edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The degree of the vertex $u \in V(G)$ is the number of edges that incident to u, and denoted by $\delta_G(u)$. The size of a graph G is the number of edges in G and denoted by $|E| = m$ and the number of vertices of G is called the order of G and denoted by $|V| = n$. The complement of G, denoted by $\overline{G}$, is a simple graph on the same set of vertices $V(G)$ in which two vertices u and v are adjacent, i.e., connected by an edge uv, $\iff$ they are not adjacent in G. Hence, $uv \in E(\overline{G}), \iff uv \notin E(G)$. Obviously $E(G) \cup E(\overline{G}) = E(K_n)$, and $\overline{m} = |E(\overline{G})| = \binom{n}{2} - m$, the degree of a vertex u in $\overline{G}$, is the number of edges incident to u, denoted by $\delta_{\overline{G}}(u) = (n-1) - \delta_G(u)$.

Proposition 2.1. [10] *Let G be a simple graph on n vertices and m edges. Then,*
$Y(\overline{G}) = n(n-1)^4 - 8m(n-1)^3 + 6(n-1)^2 M_1(G) - 4(n-1)F(G) + Y(G)$,
$\overline{Y}(G) = (n-1)F(G) - Y(G)$.

Theorem 2.1. [11] *The first and second Zagreb indices of $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$ nanotube (Fig.1) and (Fig.2) respectively, is given by*

$$M_1(VC_5C_7[p,q]) = 12p[12q+2],$$
$$M_2(VC_5C_7[p,q]) = p[216q+18],$$
$$M_1(HC_5C_7[p,q]) = p[72q+20],$$
$$M_2(HC_5C_7[p,q]) = p[108q+16].$$

3. Y-index and coindex of $VC_5C_7[p,q]$ nanotube $(p,q \geq 1)$

In this section, we compute the Y-index and coindex for line graphs of the $VC_5C_7[p,q]$ nanotubes and its molecular complement graph. Moreover, we define $Y-polynomial$ of graph G and apply it on the line graphs of the $VC_5C_7[p,q]$ nanotubes.

Theorem 3.1. *The $Y-index$ of $VC_5C_7[p,q]$ nanotube (Fig.1) is given by*

$$Y(VC_5C_7[p,q]) = p[1296q + 96].$$

Proof. By definition of the $Y-index$ $Y(G) = \sum\limits_{uv \in E(G)} \left[\delta_G^3(u) + \delta_G^3(v)\right]$, and by replacing each G with $VC_5C_7[p,q]$, which yield to $Y(VC_5C_7[p,q]) = \sum_{uv \in E(VC_5C_7[p,q])} \Big[\delta^3_{VC_5C_7[p,q]}(u) + \delta^3_{VC_5C_7[p,q]}(v)\Big]$, and the partitions of the vertex set and edge set $V(VC_5C_7[p,q])$, $E(VC_5C_7[p,q])$, of $VC_5C_7[p,q]$ nanotubes are given in (Table 1,2) respectively [11], such

that the parameter p is denoted as the number of pentagons in the first row of $VC_5C_7[p, q]$ and q is denoted as the number of repetitions. So, for any $p, q \in \mathbb{N}$, there exist $6p$ vertices and $16p$ edges in each period of $VC_5C_7[p, q]$ which are neighboring at the end of the Nano-Structure. for any graph G, its vertex set $V(G)$ and edge set $E(G)$ are divided into several partitions:
for any $r \in \mathbb{N}, 2\delta(G) \leq r \leq 2\Delta(G)$, let $E_r = e = uv \in E(G) : \delta(u) + \delta(v) = r$; for any $s \in \mathbb{N}, \delta^2(G) \leq s \leq \Delta^2(G)$, let $E_s^* = e = uv \in E(G) : \delta(u)\delta(v) = s$; for any $t \in \mathbb{N}, \delta(G) \leq t \leq \Delta(G)$, let $V_t = v = v \in V(G) : \delta(v) = t$; Then, the edge set of $VC_5C_7[p, q]$ is divided into two edge partitions based on the sum of degrees of the end vertices as:

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

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

We see that $|V(VC_5C_7[p, q])| = 16pq + 6p$ and $|E(VC_5C_7[p, q])| = 24pq + 6p$.

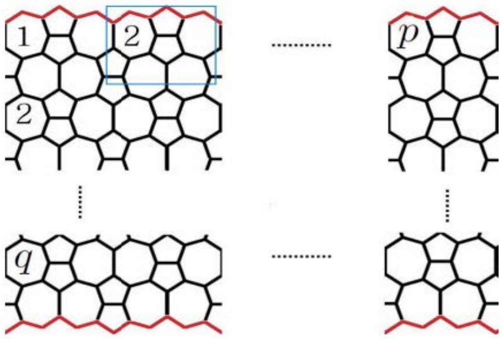

FIGURE 1. molecular graph of a $VC_5C_7[p, q]$ nanotube.

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	$3p + 3p$	$16pq$

Thus:

$$\begin{aligned} Y(VC_5C_7[p, q]) &= \sum_{uv \in E(VC_5C_7[p,q])} \left[\delta^3_{VC_5C_7[p,q]}(u) + \delta^3_{VC_5C_7[p,q]}(v)\right] \\ &= \sum_{uv \in E_6^*(VC_5C_7[p,q])} \left[\delta^3_{VC_5C_7[p,q]}(u) + \delta^3_{VC_5C_7[p,q]}(v)\right] \\ &+ \sum_{uv \in E_9^*(VC_5C_7[p,q])} \left[\delta^3_{VC_5C_7[p,q]}(u) + \delta^3_{VC_5C_7[p,q]}(v)\right] \\ &= 35|E_6^*(VC_5C_7[p, q])| + 54|E_9^*(VC_5C_7[p, q])| \\ &= 1296pq + 96p. \end{aligned}$$

□

Definition 3.1. *The Y-polynomial of graph G defined as*

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

Theorem 3.2. *The $Y-polynomial$ of $VC_5C_7[p,q]$ nanotube (Fig.1) is given by*

$$Y(VC_5C_7[p,q],x) = 6p\Big[2x^{35} + [4q-1]x^{54}\Big].$$

Proof. By definition of the Y-polynomial of graph G above. and as (Theorem 3.1) 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 (Table 1,2) respectively we have,

$$\begin{aligned}
Y(VC_5C_7[p,q],x) &= \sum_{uv\in E(VC_5C_7[p,q])} x^{[\delta^3_{VC_5C_7[p,q]}(u)+\delta^3_{VC_5C_7[p,q]}(v)]}\\
&= \sum_{uv\in E_6^*(VC_5C_7[p,q])} x^{[\delta^3_{VC_5C_7[p,q]}(u)+\delta^3_{VC_5C_7[p,q]}(v)]}\\
&+ \sum_{uv\in E_9^*(VC_5C_7[p,q])} x^{[\delta^3_{VC_5C_7[p,q]}(u)+\delta^3_{VC_5C_7[p,q]}(v)]}\\
&= |E_6^*(VC_5C_7[p,q])|x^{35} + |E_9^*(VC_5C_7[p,q])|x^{54}\\
&= 12px^{35} + [24pq-6p]x^{54}\\
&= 6p\Big[2x^{35} + [4q-1]x^{54}\Big].
\end{aligned}$$

We can also get the $Y-index$ of $VC_5C_7[p,q]$ nanotube by derivating the formula Y-polynomial of $VC_5C_7[p,q]$ nanotube above as:

$$\begin{aligned}
Y(VC_5C_7[p,q]) &= \frac{\partial Y(VC_5C_7[p,q],x)}{\partial x}|_{x=1} = \frac{\partial\Big[12px^{35} + 6p[4q-1]x^{54}\Big]}{\partial x}|_{x=1}\\
&= 1296pq + 96p.
\end{aligned}$$

□

Theorem 3.3. *The $F-index$ of $VC_5C_7[p,q]$ nanotube (Fig.1) is given by*

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

Proof. By definition of forgotten index (F-index) and Theorem (3.1). Then,

$$\begin{aligned}
F(VC_5C_7[p,q]) &= \sum_{uv\in E(VC_5C_7[p,q])} \Big[\delta^2_{VC_5C_7[p,q]}(u) + \delta^2_{VC_5C_7[p,q]}(v)\Big]\\
&= \sum_{uv\in E_6^*(VC_5C_7[p,q])} \Big[\delta^2_{VC_5C_7[p,q]}(u) + \delta^2_{VC_5C_7[p,q]}(v)\Big]\\
&+ \sum_{uv\in E_9^*(VC_5C_7[p,q])} \Big[\delta^2_{VC_5C_7[p,q]}(u) + \delta^2_{VC_5C_7[p,q]}(v)\Big]\\
&= 13|E_6^*(VC_5C_7[p,q])| + 18|E_9^*(VC_5C_7[p,q])|\\
&= 48p[1+9q].
\end{aligned}$$

□

Corollary 3.1. *The $Y-$ index of complement $VC_5C_7[p,q]$ nanotube (Fig.1) is given by*

$$\begin{aligned} Y(\overline{VC_5C_7[p,q]}) &= [16pq+6p](16pq+6p-1)^4 - 8(24pq+6p)(16pq+6p-1)^3 \\ &+ 6(16pq+6p-1)^2[144pq+24p] \\ &- 4(16pq+6p-1)[48p+432pq]+1296pq+96p. \end{aligned}$$

Proof. By (Proposition 2.1) we have

$$Y(\overline{G}) = n(n-1)^4 - 8m(n-1)^3 + 6(n-1)^2M_1(G) - 4(n-1)F(G) + Y(G),$$

And $F(VC_5C_7[p,q]) = 48p[1+9q]$ given in (Theorem 3.3)above. $M_1(VC_5C_7[p,q]) = 144pq+24p$ and the partitions of the vertex set and edge set of $(VC_5C_7[p,q])$ nanotubes are given in [11].

$$\sum|V(VC_5C_7[p,q])| = 16pq+6p, \qquad \sum|E(VC_5C_7[p,q])| = 24pq+6p$$

and $Y(VC_5C_7[p,q]) = 1296pq+96p$ given in Theorem (3.1)above. Thus

$$\begin{aligned} Y(\overline{VC_5C_7[p,q]}) &= \sum|V(VC_5C_7[p,q])|\Big(\sum|V(VC_5C_7[p,q])|-1\Big)^4 \\ &- 8\sum|E(VC_5C_7[p,q])|\Big(\sum|V(VC_5C_7[p,q])|-1\Big)^3 \\ &+ 6\Big(\sum|V(VC_5C_7[p,q])|-1\Big)^2 M_1(VC_5C_7[p,q]) \\ &- 4\Big(\sum|V(VC_5C_7[p,q])|-1\Big)F(VC_5C_7[p,q]) + Y(VC_5C_7[p,q]) \\ &= [16pq+6p](16pq+6p-1)^4 - 8(24pq+6p)(16pq+6p-1)^3 \\ &+ 6(16pq+6p-1)^2[144pq+24p] \\ &- 4(16pq+6p-1)[48p+432pq]+1296pq+96p. \end{aligned}$$

□

Corollary 3.2. *The $Y-$ coindex of $VC_5C_7[p,q]$ nanotube (Fig.1) is given by*

$$\overline{Y}(VC_5C_7[p,q]) = 48p[9q+1][p(16q+6)-1] - p[1296q+96].$$

Proof. By (Proposition 2.1) we have $\overline{Y}(G) = (n-1)F(G) - Y(G)$, $F(VC_5C_7[p,q]) = 48p[1+9q]$ given in Theorem (3.3) and $Y(VC_5C_7[p,q]) = 1296pq+96p$ given in Theorem (3.1)above. and since $n = \sum|V(VC_5C_7[p,q])| = 16pq+6p$. Then,

$$\begin{aligned} \overline{Y}(VC_5C_7[p,q]) &= \Big(\sum|V(VC_5C_7[p,q])|-1\Big)F(VC_5C_7[p,q]) - Y(VC_5C_7[p,q]) \\ &= 48p[16pq+6p-1][1+9q] - 1296pq - 96p. \end{aligned}$$

□

Proposition 3.1. *Let G be a simple graph on n vertices and m edges. Then,*
$\overline{Y}(\overline{G}) = 4m(n-1)^3 - 3(n-1)^2M_1(G) + 3(n-1)F(G) - Y(G)$.

Corollary 3.3. *The $Y-$coindex of complement $VC_5C_7[p,q]$ nanotube (Fig.1) is given by*

$$\begin{aligned} \overline{Y}(\overline{VC_5C_7[p,q]}) &= 4[24pq+6p]\Big[16pq+6p-1\Big])^3 - 3[144pq+24p]\Big[16pq+6p-1\Big]^2 \\ &+ 3\Big(16pq+6p-1\Big)[48p(1+9q)] - 1296pq - 96p. \end{aligned}$$

Proof. By (Proposition 3.1) we have

$$\overline{Y}(\overline{G}) = 4m(n-1)^3 - 3(n-1)^2 M_1(G) + 3(n-1)F(G) - Y(G),$$

$F(VC_5C_7[p,q]) = 48p[1+9q]$ given in (Theorem 3.3) and $Y(VC_5C_7[p,q]) = 1296pq + 96p$ given in (Theorem 3.1)above. and as (Corollary 3.1) the partitions of the vertex set and edge set of $(VC_5C_7[p,q])$ nanotubes. Then,

$$\begin{aligned}
\overline{Y}(\overline{VC_5C_7[p,q]}) &= 4\sum|E(VC_5C_7[p,q])|\Big[\sum|V(VC_5C_7[p,q])|-1\Big]^3 \\
&- 3\Big[\sum|V(VC_5C_7[p,q])|-1\Big]^2 M_1(VC_5C_7[p,q]) \\
&+ 3\Big[\sum|V(VC_5C_7[p,q])|-1\Big]F(VC_5C_7[p,q]) - Y(VC_5C_7[p,q]) \\
&= 4[24pq+6p]\Big[16pq+6p-1\Big])^3 - 3[144pq+24p]\Big[16pq+6p-1\Big]^2 \\
&+ 3\Big(16pq+6p-1\Big)[48p(1+9q)] - 1296pq - 96p.
\end{aligned}$$

□

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

p	q	$M_1(H)$	$M_2(H)$	$F(H)$	$Y(H)$	$\overline{Y}(H)$
1	1	168	234	480	1392	8.688×10^3
1	2	312	450	912	2688	31.056×10^3
1	3	456	666	1344	3984	67.248×10^3
2	1	336	468	960	2784	38.496×10^3
2	2	624	900	1824	5376	131.424×10^3
2	3	912	1332	2688	7968	279.648×10^3
3	1	504	702	1440	4176	89.424×10^3
3	2	936	1350	2736	8064	301.104×10^3
3	3	1368	1996	4032	11952	637.200×10^3

In (Table 3.) some index and coindex values of $VC_5C_7[p,q]$ nanotubes. formulas reported in (Theorem 3.1), (Theorem 3.2) and (Corollary 3.2) for the $VC_5C_7[p,q]$ nanotube. In table it show that values of first and second Zagreb indices, $F-index$, $Y-index$ and $Y-coindex$ are in increasing order as the values of p,q increase.

4. Y-INDEX AND COINDEX OF $VC_5C_7[p,q]$ NANOTUBE $(p,q \geq 1)$

In this section, we compute the Y-index and coindex for line graphs of the $HC_5C_7[p,q]$ nanotubes and its molecular complement graph. Moreover, we apply $Y-polynomial$ on the line graphs of the $HC_5C_7[p,q]$ nanotubes.

Theorem 4.1. *The $Y-index$ of $HC_5C_7[p,q]$ nanotube (Fig.2) is given by*

$$Y(HC_5C_7[p,q]) = p[648q+80]$$

Proof. By definition of the $Y-index$ and by [11] 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 (Table 4,5) respectively, such that the parameter p is denoted as the number of pentagons in the first row of $HC_5C_7[p,q]$ and q is denoted as the number of repetitions. So, for any $p,q \in \mathbb{N}$,

there exist $12p$ edges and $8p$ vertices in each period of $HC_5C_7[p,q]$ which are adjacent at the end of the Nano-Structure. for any graph G, its vertex set $V(G)$ and edge set $E(G)$ are divided into several partitions:
for any $r \in \mathbb{N}, 2\delta(G) \leq r \leq 2\Delta(G)$, let $E_r = e = uv \in E(G) : \delta(u)+\delta(v) = r$; for any $s \in \mathbb{N}, \delta^2(G) \leq s \leq \Delta^2(G)$, let $E^*_s = e = uv \in E(G) : \delta(u)\delta(v) = s$; for any $t \in \mathbb{N}, \delta(G) \leq t \leq \Delta(G)$, let $V_t = v = v \in V(G) : \delta(v) = t$; Then, 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:

$$E_4(HC_5C_7[p,q]) = E^*_4 = \{e = uv \in E(HC_5C_7[p,q]) : \delta(u) = 2, \delta(v) = 2\},$$

$$E_5(HC_5C_7[p,q]) = E^*_6 = \{e = uv \in E(HC_5C_7[p,q]) : \delta(u) = 2, \delta(v) = 3\},$$

$$E_6(HC_5C_7[p,q]) = E^*_9 = \{e = uv \in E(HC_5C_7[p,q]) : \delta(u) = 3, \delta(v) = 3\},$$

We see that $|V(HC_5C_7[p,q])| = 8pq + 5p$ and $|E(HC_5C_7[p,q])| = 12pq + 5p$.

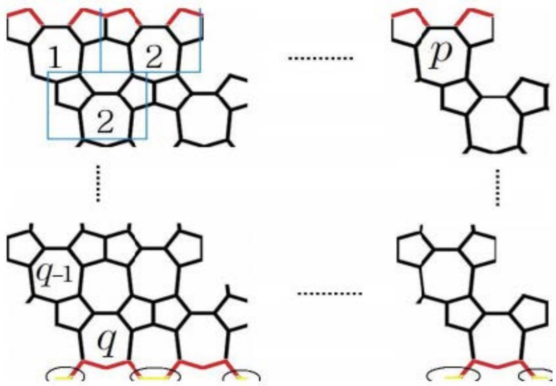

FIGURE 2. molecular graph of a $HC_5C_7[p,q]$ nanotube.

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	$5p$	$8pq$

Thus:

$$\begin{aligned}
Y(HC_5C_7[p,q]) &= \sum_{uv\in E(HC_5C_7[p,q]} \Big[\delta^3_{HC_5C_7[p,q]}(u)+\delta^3_{HC_5C_7[p,q]}(v)\Big] \\
&= \sum_{uv\in E_4^*(HC_5C_7[p,q])} \Big[\delta^3_{HC_5C_7[p,q]}(u)+\delta^3_{HC_5C_7[p,q]}(v)\Big] \\
&+ \sum_{uv\in E_6^*(HC_5C_7[p,q])} \Big[\delta^3_{HC_5C_7[p,q]}(u)+\delta^3_{HC_5C_7[p,q]}(v)\Big] \\
&+ \sum_{uv\in E_9^*(HC_5C_7[p,q])} \Big[\delta^3_{HC_5C_7[p,q]}(u)+\delta^3_{HC_5C_7[p,q]}(v)\Big] \\
&= 16|E_4^*(HC_5C_7[p,q])|+35|E_6^*(HC_5C_7[p,q])|+54|E_9^*(HC_5C_7[p,q])| \\
&= 16p+280p+54[12pq-4p].
\end{aligned}$$

□

Theorem 4.2. *The $Y-polynomial$ of $HC_5C_7[p,q]$ nanotube (Fig.2) is given by*

$$Y(HC_5C_7[p,q],x)=p\Big[x^{16}+8x^{35}+[12q-4]x^{54}\Big].$$

Proof. By definition of the $Y-polynomial$ of graph G above. and as (Theorem 4.1) the partitions of the vertex set and edge set of $(HC_5C_7[p,q])$ nanotubes. Thus,

$$\begin{aligned}
Y(HC_5C_7[p,q],x) &= \sum_{uv\in E(HC_5C_7[p,q])} x^{[\delta^3_{HC_5C_7[p,q]}(u)+\delta^3_{HC_5C_7[p,q]}(v)]} \\
&= \sum_{uv\in E_4^*(HC_5C_7[p,q])} x^{[\delta^3_{HC_5C_7[p,q]}(u)+\delta^3_{HC_5C_7[p,q]}(v)]} \\
&+ \sum_{uv\in E_6^*(HC_5C_7[p,q])} x^{[\delta^3_{HC_5C_7[p,q]}(u)+\delta^3_{HC_5C_7[p,q]}(v)]} \\
&+ \sum_{uv\in E_9^*(HC_5C_7[p,q])} x^{[\delta^3_{HC_5C_7[p,q]}(u)+\delta^3_{HC_5C_7[p,q]}(v)]} \\
&= |E_4^*(HC_5C_7[p,q])|x^{16}+|E_6^*(HC_5C_7[p,q])|x^{35}+|E_9^*(HC_5C_7[p,q])|x^{54} \\
&= px^{16}+8px^{35}+[12pq-4p]x^{54} \\
&= p\Big[x^{16}+8x^{35}+[12q-4]x^{54}\Big].
\end{aligned}$$

We can also get the $Y-index$ of $HC_5C_7[p,q]$ nanotube by derivating the formula $Y-polynomial$ of $HC_5C_7[p,q]$ nanotube above as:

$$\begin{aligned}
Y(HC_5C_7[p,q]) &= \frac{\partial Y(HC_5C_7[p,q],x)}{\partial x}|_{x=1} = \frac{\partial\Big[px^{16}+8px^{35}+p[12q-4]x^{54}\Big]}{\partial x}|_{x=1} \\
&= 80p+648pq.
\end{aligned}$$

□

Theorem 4.3. *The $F-index$ of $HC_5C_7[p,q]$ nanotube (Fig.2) is given by*

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

Proof. By definition of forgotten index (F-index) and as (Theorem 4.1) 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 (Table 4,5) respectively. Then,

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

□

Corollary 4.1. *The Y-index of complement $HC_5C_7[p,q]$ nanotube (Fig.2) is given by*

$$\begin{aligned}
Y(\overline{HC_5C_7[p,q]}) &= [8pq+5p](8pq+5p-1)^4 - 8(12pq+5p)(8pq+5p-1)^3 \\
&+ 6(8pq+5p-1)^2[72pq+20p] \\
&- 4(8pq+5p-1)[216pq+40p] + 80p + 648pq.
\end{aligned}$$

Proof. By (Proposition 2.1) we have

$$Y(\overline{G}) = n(n-1)^4 - 8m(n-1)^3 + 6(n-1)^2M_1(G) - 4(n-1)F(G) + Y(G),$$

And $F(HC_5C_7[p,q]) = 216pq+40p$ given in Theorem (4.3), $M_1(HC_5C_7[p,q]) = 72pq+20p$ and the partitions of the vertex set and edge set of $(HC_5C_7[p,q])$ nanotubes are given in [11].

$$\sum |V(HC_5C_7[p,q])| = 8pq+5p, \qquad \sum |E(HC_5C_7[p,q])| = 12pq+5p$$

and $Y(HC_5C_7[p,q]) = 80p + 648pq$ given in (Theorem 4.1) above. Then,

$$\begin{aligned}
Y(\overline{HC_5C_7[p,q]}) &= \sum |V(HC_5C_7[p,q])|\Big(\sum |V(HC_5C_7[p,q])| - 1\Big)^4 \\
&- 8\sum |E(HC_5C_7[p,q])|\Big(\sum |V(HC_5C_7[p,q])| - 1\Big)^3 \\
&+ 6\Big(\sum |V(HC_5C_7[p,q])| - 1\Big)^2 M_1(HC_5C_7[p,q]) \\
&- 4\Big(\sum |V(HC_5C_7[p,q])| - 1\Big)F(HC_5C_7[p,q]) + Y(HC_5C_7[p,q]) \\
&= [8pq+5p](8pq+5p-1)^4 - 8(12pq+5p)(8pq+5p-1)^3 \\
&+ 6(8pq+5p-1)^2[72pq+20p] \\
&- 4(8pq+5p-1)[216pq+40p] + 80p + 648pq.
\end{aligned}$$

□

Corollary 4.2. *The Y-coindex of $HC_5C_7[p,q]$ nanotube (Fig.2) is given by*

$$\overline{Y}(HC_5C_7[p,q]) = p[216q+40][p(8q+5)-1] - p[648q+80].$$

Proof. By (Proposition 2.1) we have $\overline{Y}(G) = (n-1)F(G) - Y(G)$, and by (Corollary 4.1) we obtian,

$$\begin{aligned}\overline{Y}(HC_5C_7[p,q]) &= \Big(\sum |V(HC_5C_7[p,q])| - 1\Big)F(HC_5C_7[p,q]) - Y(HC_5C_7[p,q]) \\ &= [8pq+5p-1][216pq+40p] - 80p - 648pq.\end{aligned}$$

□

Corollary 4.3. *The Y-coindex of complement $HC_5C_7[p,q]$ nanotube (Fig.2) is given by*

$$\begin{aligned}\overline{Y}(\overline{HC_5C_7[p,q]}) &= 4[12pq+5p]\Big(8pq+5p-1\Big)^3 - 3\Big(8pq+5p-1\Big)^2[72pq+20p] \\ &+ 3\Big(8pq+5p-1\Big)[216pq+40p] - 80p - 648pq.\end{aligned}$$

Proof. By (Proposition 3.1) we have

$$\overline{Y}(\overline{G}) = 4m(n-1)^3 - 3(n-1)^2M_1(G) + 3(n-1)F(G) - Y(G),$$

$F(HC_5C_7[p,q]) = 216pq + 40p$ given in (Theorem 4.3) above. and $Y(HC_5C_7[p,q]) = 80p + 648pq$ given in (Theorem 4.1), and since

$$n = \sum |V(HC_5C_7[p,q])| = 8pq+5p, \qquad m = \sum |E(HC_5C_7[p,q])| = 12pq+5p$$

Then,

$$\begin{aligned}\overline{Y}(\overline{HC_5C_7[p,q]}) &= 4\sum |E(HC_5C_7[p,q])|\Big(\sum |V(HC_5C_7[p,q])| - 1\Big)^3 \\ &- 3\Big(\sum |V(HC_5C_7[p,q])| - 1\Big)^2 M_1(HC_5C_7[p,q]) \\ &+ 3\Big(\sum |V(HC_5C_7[p,q])| - 1\Big)F(HC_5C_7[p,q]) - Y(HC_5C_7[p,q]) \\ &= 4[12pq+5p]\Big(8pq+5p-1\Big)^3 - 3\Big(8pq+5p-1\Big)^2[72pq+20p] \\ &+ 3\Big(8pq+5p-1\Big)[216pq+40p] - 80p - 648pq.\end{aligned}$$

□

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

p	q	$M_1(G)$	$M_2(G)$	$F(G)$	$Y(G)$	$\overline{Y}(G)$
1	1	92	124	256	728	23.44×10^2
1	2	164	232	472	1376	80.64×10^2
1	3	236	340	688	2024	172.40×10^2
2	1	184	248	512	1456	113.44×10^2
2	2	328	464	944	2752	359.52×10^2
2	3	472	680	1376	4048	743.84×10^2
3	1	276	372	768	2184	27.00×10^3
3	2	492	696	1416	4128	836.64×10^2
3	3	708	1020	2064	6072	171.432×10^3

In (Table 6.) some index and coindex values of $HC_5C_7[p,q]$ nanotubes. formulas reported in (Theorem 4.1), (Theorem 4.3) and (Corollary 4.2) for the $HC_5C_7[p,q]$ nanotube. In table it show that values of first and second Zagreb indices, $F-index$, $Y-index$ and $Y-coindex$ are in increasing order as the values of p,q increase.

5. Conclusions

The present study has computed the Y-index and coindex of line graphs of the $VC_5C_7[p,q]$, $HC_5C_7[p,q]$ nanotubes and their molecular complement graphs. The study also has defined Y-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. Our obtained explicit formulae can correlate the chemical structure of molecular graph of nanotubes to information about their physical structure.

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