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Research Article

The *Y*-Index of Some Complement Graph Structures and Their Applications of Nanotubes and Nanotorus

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Topological descriptors play a significant role in chemical nanostructures. These topological measures have explicit chemical uses in chemistry, medicine, biology, and computer sciences. This study calculates the *Y*-index of some graphs and complements graph operations such as join, tensor and Cartesian and strong products, composition, disjunction, and symmetric difference between two simple graphs. Moreover, the *Y*-polynomial of titania nanotubes and the formulae for the *Y*-index, *Y*-polynomial, *F*-index, *F*-polynomial, and *Y*-coindex of the $HAC_5C_7[q, p]$ and $HAC_5C_6C_7[q, p]$ nanotubes and their molecular complement graphs have been investigated.

1. Introduction

Topological indices are useful molecular descriptions in the field of chemical graph theory to establish the structural property and structural-activity relationship that describes chemical component structures and helps predict certain chemical-physical properties [1, 2]. There are many topological descriptors that are proposed and studied based on degree, distance, eigenvalue, matching, and mixed and other parameters of graphs [3].

The importance of computing the complement graphs is to identify adjacent intervals and thus develop the data structure to process them efficiently [4]. There have been many studies that have improved the complexity of time problems related to dense graphs and complement graphs (see [5–7]). On some problems, the computational time may be reduced by using the algorithms of complement graphs. For example, Ito and Yokoyama explored the linear time resolution of several storage-based problems [8]. They have looked at storage methods for representing nondirected graphs and maintaining the graphs and their complement graphs in the data structure. They demonstrated that the order of legal nodes and sparse subgraphs that preserve the connectivity properties of a specific graph of the complement graph can be found in linear time and that the width-first search tree and the depth-first search tree of the complement graph of a specific graph can be constructed in linear time.

In our study, we consider a finite connected and an undirected graph Γ with $E(\Gamma)$ edges and $V(\Gamma)$ vertices. The vertex degree of $\mu \in V(\Gamma)$ is the number of edges connected to μ and is represented by $\delta_{\Gamma}(\mu)$. The size of a graph Γ is the number of edges in Γ and is expressed as $|E| = q$ and the number of vertices of Γ is called the order of Γ and is represented by $|V| = p$. The complement of a graph Γ, indicated by $\overline{\Gamma}$, is a graph on the same set $V(\Gamma)$ such that every two vertices μ and ν are adjacent to each other, i.e., they are connected by an edge $\mu\nu$ if, and only if, they are not adjacent to each other in Γ. Then, $\mu\nu \in E(\overline{\Gamma}) \Rightarrow \mu\nu \notin E(\Gamma)$. Consequently, $E(\Gamma) \cup E(\overline{\Gamma}) = E(K_p)$ and $\overline{q} = |E(\overline{\Gamma})| = \binom{p}{2} - q$, the degree of a vertex μ in $\overline{\Gamma}$, is the number of edges connected to μ and is defined by $\delta_{\overline{\Gamma}}(\mu) = (p-1) - \delta_\Gamma(\mu)$. For example, the benzene graph and its complement graph are shown in Figure 1. The 1st and 2nd Zagreb indices are considered to be one of the oldest descriptors of the graph defined in 1972 by Gutman and Trinajstić [9]. They are defined for a graph Γ as follows:

$$\begin{aligned} M_1(\Gamma) &= \sum_{\mu\nu \in E(\Gamma)} \left[\delta_\Gamma(\mu) + \delta_\Gamma(\nu)\right], \\ M_2(\Gamma) &= \sum_{\mu\nu \in E(\Gamma)} \delta_\Gamma(\mu)\,\delta_\Gamma(\nu). \end{aligned} \tag{1}$$

Došlić [10] defined Zagreb coindices as follows:

$$\begin{aligned} \overline{M}_1(\Gamma) &= \sum_{\mu\nu \in E(\Gamma)} \left[\delta_\Gamma(\mu) + \delta_\Gamma(\nu)\right], \\ \overline{M}_2(\Gamma) &= \sum_{\mu\nu \notin E(\Gamma)} \delta_\Gamma(\mu)\,\delta_\Gamma(\nu). \end{aligned} \tag{2}$$

Furtula et al. in 2015 [11, 12] presented the Forgotten index (F-index) that is defined as follows:

$$\begin{aligned} F(\Gamma) &= \sum_{\nu \in V(\Gamma)} \delta_\Gamma{}^3(\nu) \\ &= \sum_{\mu\nu \in E(\Gamma)} \left(\delta_\Gamma{}^2(\mu) + \delta_\Gamma{}^2(\mu)\right). \end{aligned} \tag{3}$$

De et al. [13] introduced a new descriptor denoted by F-coindex, defined as follows:

$$\overline{F}(\Gamma) = \sum_{\mu\nu \notin E(\Gamma)} \left(\delta_\Gamma{}^2(\mu) + \delta_\Gamma{}^2(\nu)\right). \tag{4}$$

Alameri et al. [14, 15] in 2020 defined new degree-based descriptors, denoted by the (Y – index) and (Y – coindex), and they are, respectively, defined as follows:

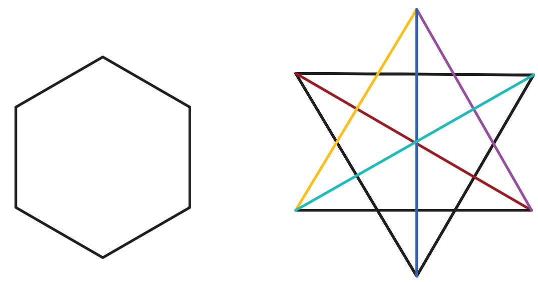
$$\begin{aligned} Y(\Gamma) &= \sum_{\mu\nu \in E(\Gamma)} \left[\delta_\Gamma^3(\mu) + \delta_\Gamma^3(\nu)\right], \\ \overline{Y}(\Gamma) &= \sum_{\mu\nu \notin E(\Gamma)} \left[\delta_\Gamma^3(\mu) + \delta_\Gamma^3(\nu)\right]. \end{aligned} \tag{5}$$

Also, in the same papers, the (Y – index) and (Y – coindex) formulae of the graph and complement graph Γ are investigated and defined as follows:

$$\begin{aligned} Y(\overline{\Gamma}) = {} & p(p-1)^4 - 8q(p-1)^3 + 6(p-1)^2 M_1(\Gamma) \\ & - 4(p-1)F(\Gamma) + Y(\Gamma), \end{aligned} \tag{6}$$

$$\overline{Y}(\Gamma) = (p-1)F(\Gamma) - Y(\Gamma). \tag{7}$$

The first general Zagreb index introduced by Li and Zheng is as follows [16]:



Γ Γ–complement

Figure 1: The benzene graph and its complement graph.

$$\begin{aligned} M_1^{\alpha+1}(G) &= \sum_{\nu \in V(G)} \delta_G^{\alpha+1}(\nu) \\ &= \sum_{\mu\nu \in E(G)} \delta_G^{\alpha}(\mu) + \delta_G^{\alpha}(\nu). \end{aligned} \tag{8}$$

Several studies have been conducted on various topological indices in different graph operations. De et al. [13] introduced the F-index and the F-coindex in several graph operations, such as join, union, Cartesian and corona products, composition, tensor and strong products, symmetric difference, and disjunction in graphs. Another study by Veylaki et al. [17] in 2015 derived some exact formulae for calculating the third and hyper-Zagreb coindices of certain graph operations. Khalifeh et al. [18] and Ashrafi et al. [19], respectively, computed the 1st and 2nd Zagreb indices and coindices of some operations on graphs. Das et al. [20] obtained some exact formulae for computing upper bounds for multiplicative Zagreb indices for some operations on graphs. In 2014, De et al. [21], in different graph operations, have obtained explicit formulae of the connective eccentric index. Azari and Iranmanesh [22] presented exact formulae for the eccentric distance sum of some operations on graph. Alameri et al. [14, 15] computed the Y-index and coindex of the Cartesian product $\Gamma_1 \times \Gamma_2$, composition $\Gamma_1 \circ \Gamma_2$, disjunction $\Gamma_1 \vee \Gamma_2$, symmetric difference $\Gamma_1 \oplus \Gamma_2$, tensor product $\Gamma_1 \otimes \Gamma_2$, and strong product $\Gamma_1 * \Gamma_2$ of two undirected and connected graphs. Alsharafi et al. [23–25] studied the first, second, forgotten, and second hyper-Zagreb indices of some graph and complement operations on the graph. This paper will further explore the behavior of the Y-index for joining two connected graphs and the Y-index of the various graph operations to supplement the graph and apply the results to find the Y-index of some certain nanostructures. However, many other graphs operations do not cover here. For further research, it is possible to consider the Y-index and Y-coindex of various other graphs and the complement graph operations.

Now, we present a few definitions of operations that we would be using in our results as follows:

The tensor product $(\Gamma_1 \otimes \Gamma_2)$ of Γ_1 and Γ_2 graphs is the graph with the $V(\Gamma_1) \times V(\Gamma_2)$ vertex, set where (μ_1, ν_1) is adjacent with (μ_2, ν_2) iff μ_1 is adjacent with μ_2 and ν_1 is adjacent with ν_2.

The join $(\Gamma_1 + \Gamma_2)$ of Γ_1 and Γ_2 graphs with disjoint $V(\Gamma_1)$ and $V(\Gamma_2)$ sets and edge $E(\Gamma_1)$ and $E(\Gamma_1)$ sets is the union $\Gamma_1 \cup \Gamma_2$ graph, both with all the edges that join $V(\Gamma_1)$ and $V(\Gamma_2)$ with each other.

The Cartesian product $(\Gamma_1 \times \Gamma_2)$ of Γ_1 and Γ_2 graphs with disjoint $V(\Gamma_1)$ and $V(\Gamma_2)$ vertex sets and $E(\Gamma_1)$ and $E(\Gamma_1)$ edge sets is the graph with the vertex set $V(\Gamma_1 \times \Gamma_2) = V(\Gamma_1) \times V(\Gamma_2)$, where (μ_1, ν_1) is adjacent with (μ_2, ν_2) whenever $\mu_1 = \nu_1$ and μ_2 is adjacent with ν_2 or $\mu_2 = \nu_2$ and μ_1 is adjacent with ν_1 such that $\mu_1, \mu_2 \in V(\Gamma_1)$ and $\nu_1, \nu_2 \in V(\Gamma_2)$.

The composition $(\Gamma_1 \Gamma_2)$ of Γ_1 and Γ_2 graphs with disjoint $V(\Gamma_1)$ and $V(\Gamma_2)$ vertex sets and $E(\Gamma_1)$ and $E(\Gamma_1)$ edge sets is the graph with the $V(\Gamma_1) \times V(\Gamma_2)$ vertex set, where (μ_1, μ_2) is adjacent with (ν_1, ν_2), whenever μ_1 is adjacent with ν_1 or $\mu_1 = \nu_1$ and μ_2 is adjacent with ν_2 such that $\mu_1, \mu_2 \in V(\Gamma_1)$ and $\nu_1, \nu_2 \in V(\Gamma_2)$.

The strong product $(\Gamma_1 * \Gamma_2)$ of Γ_1 and Γ_2 graphs with $V(\Gamma_1)$ and $V(\Gamma_2)$ vertex sets and $E(\Gamma_1)$ and $E(\Gamma_1)$ edge sets is the graph with the vertex set $V(\Gamma_1) \times V(\Gamma_2)$, where (μ_1, ν_1) is adjacent with (μ_2, ν_2) whenever $\nu_1 = \nu_2$ and μ_1 is adjacent with μ_2 or $\mu_1 = \mu_2$ and ν_1 is adjacent with ν_2 or μ_1 is adjacent with μ_2 and ν_1 is adjacent with ν_2.

The disjunction $(\Gamma_1 \vee \Gamma_2)$ of Γ_1 and Γ_2 graphs with $V(\Gamma_1)$ and $V(\Gamma_2)$ vertex sets and $E(\Gamma_1)$ and $E(\Gamma_1)$ edge sets is the graph with the vertex $V(\Gamma_1) \times V(\Gamma_2)$ set, where (μ_1, ν_1) is adjacent with (μ_2, ν_2) whenever $\mu_1\mu_2 \in E(\Gamma_1)$ or $\nu_1\nu_2 \in E(\Gamma_2)$.

The symmetric difference $(\Gamma_1 \oplus \Gamma_2)$ of Γ_1 and Γ_2 graphs with vertex $V(\Gamma_1)$ and $V(\Gamma_2)$ sets and $E(\Gamma_1)$ and $E(\Gamma_1)$ edge sets is the graph with the vertex set $V(\Gamma_1) \times V(\Gamma_2)$, where (μ_1, μ_2) is adjacent with (ν_1, ν_2) whenever $\mu_1\nu_1 \in E(\Gamma_1)$ or $\mu_2\nu_2 \in E(\Gamma_2)$ but not both.

2. Main Results

In this section, we examine the Y-index for the join of two graphs and the Y-index of the binary operations of various complement graphs such as the tensor and the Cartesian and strong product, the join, the composition, the disjunction, and the symmetric difference of the two graphs. In addition, we obtained the formulae for the Y-polynomial and Y-index of some nanotubes and nanotorus and their molecular complement graph.

2.1. The Y-Index of Some Complement Graph Operations. In this subsection, we compute the Y-Index of various complement graph operations as the following theorems.

Theorem 1. *Let Γ_1 and Γ_2 be two two undirected connected graphs with p_1, p_2 vertices and q_1, q_2 edges, then*

$$\begin{aligned} Y(\overline{\Gamma_1 \otimes \Gamma_2}) &= p_1p_2(p_1p_2-1)^4 - 16q_1q_2(p_1p_2-1)^3 + 6(p_1p_2-1)^2 M_1(\Gamma_1)M_1(\Gamma_2) \\ &\quad - 4(p_1p_2-1)F(\Gamma_1)F(\Gamma_2) + Y(\Gamma_1)Y(\Gamma_2). \end{aligned} \tag{9}$$

Proof. By equation (6) and since $M_1(\Gamma_1 \otimes \Gamma_2) = M_1(\Gamma_1) M_1(\Gamma_2)$, $F(\Gamma_1 \otimes \Gamma_2) = F(\Gamma_1)F(\Gamma_2)$, and $Y(\Gamma_1 \otimes \Gamma_2) = Y(\Gamma_1)Y(\Gamma_2)$ are given in [14, 26, 27], respectively, then

$$\begin{aligned} Y(\overline{\Gamma_1 \otimes \Gamma_2}) &= |V(\Gamma_1 \otimes \Gamma_2)|\left(|V(\Gamma_1 \otimes \Gamma_2)|-1\right)^4 - 8|E(\Gamma_1 \otimes \Gamma_2)|\left(|V(\Gamma_1 \otimes \Gamma_2)|-1\right)^3 + 6\left(|V(\Gamma_1 \otimes \Gamma_2)|-1\right)^2 M_1(\Gamma_1 \otimes \Gamma_2) \\ &\quad - 4\left(|V(\Gamma_1 \otimes \Gamma_2)|-1\right)F(\Gamma_1 \otimes \Gamma_2) + Y(G_1 \otimes G_2) \\ &= p_1p_2(p_1p_2-1)^4 - 16q_1q_2(p_1p_2-1)^3 + 6(p_1p_2-1)^2 M_1(\Gamma_1)M_1(\Gamma_2) \\ &\quad - 4(p_1p_2-1)F(\Gamma_1)F(\Gamma_2) + Y(\Gamma_1)Y(\Gamma_2). \end{aligned} \tag{10}$$

□

Theorem 2. *The $Y-$ index of $(\Gamma_1 + \Gamma_2)$ is given by*

$$\begin{aligned} Y(\Gamma_1 + \Gamma_2) &= Y(\Gamma_1) + 4p_2F(\Gamma_1) + 6p_2^2 M_1(\Gamma_1) + 8q_1p_2^3 + p_1p_2^4 \\ &\quad + Y(\Gamma_2) + 4p_1F(\Gamma_2) + 6p_1^2 M_1(\Gamma_2) + 8q_2p_1^3 + p_2p_1^4. \end{aligned} \tag{11}$$

Proof. By definitions of the join and the $(Y-\text{index})$, we have

$$\begin{aligned} Y(\Gamma_1+\Gamma_2) &= \sum_{\mu\nu\in E(\Gamma_1+\Gamma_2)} \left[\delta^3_{\Gamma_1+\Gamma_2}(\mu)+\delta^3_{\Gamma_1+\Gamma_2}(\nu)\right] \\ &= \sum_{\mu\nu\in E(\Gamma_1)} \left[\delta^3_{\Gamma_1+\Gamma_2}(\mu)+\delta^3_{\Gamma_1+\Gamma_2}(\nu)\right] + \sum_{\mu\nu\in E(\Gamma_2)} \left[\delta^3_{\Gamma_1+\Gamma_2}(\mu)+\delta^3_{\Gamma_1+\Gamma_2}(\nu)\right] \\ &\quad + \sum_{\mu\in V(\Gamma_1)}\sum_{\nu\in V(\Gamma_2)} \left[\delta^3_{\Gamma_1+\Gamma_2}(\mu)+\delta^3_{\Gamma_1+\Gamma_2}(\nu)\right] \\ &= \sum_{\mu\nu\in E(\Gamma_1)} \left[\left(\delta_{\Gamma_1}(\mu)+p_2\right)^3+\left(\delta_{\Gamma_1}(\nu)+p_2\right)^3\right] \\ &\quad + \sum_{\mu\nu\in E(\Gamma_2)} \left[\left(\delta_{\Gamma_2}(\mu)+p_1\right)^3+\left(\delta_{\Gamma_2}(\nu)+p_1\right)^3\right] \\ &\quad + \sum_{\mu\in V(\Gamma_1)}\sum_{\nu\in V(\Gamma_2)} \left[\left(\delta_{\Gamma_1}(\mu)+p_2\right)^3+\left(\delta_{\Gamma_2}(\nu)+p_1\right)^3\right] \\ &= \sum_{\mu\nu\in E(\Gamma_1)} \left[\delta^3_{\Gamma_1}(\mu)+\delta^3_{\Gamma_1}(\nu)+3p_2\left(\delta^2_{\Gamma_1}(\mu)+\delta^2_{\Gamma_1}(\nu)\right)+3p_2^2\left(\delta_{\Gamma_1}(\mu)+\delta_{\Gamma_1}(\nu)\right)+2p_2^3\right] \\ &\quad + \sum_{\mu\nu\in E(\Gamma_2)} \left[\delta^3_{\Gamma_2}(\mu)+\delta^3_{\Gamma_2}(\nu)+3p_1\left(\delta^2_{\Gamma_2}(\mu)+\delta^2_{\Gamma_2}(\nu)\right)+3p_1^2\left(\delta_{\Gamma_2}(\mu)+\delta_{G_2}(\nu)\right)+2p_1^3\right] \\ &\quad + \sum_{\mu\in V(\Gamma_1)}\sum_{\nu\in V(\Gamma_2)} \left[\delta^3_{\Gamma_1}(\mu)+3p_2\delta^2_{\Gamma_1}(\mu)+3p_2^2\delta_{\Gamma_1}(\mu)+p_2^3\delta^3_{\Gamma_2}(\nu)+3p_1\delta^2_{\Gamma_2}(\nu)+3p_1^2\delta_{\Gamma_2}(\nu)+p_1^3\right] \\ &= Y(\Gamma_1)+3p_2F(\Gamma_1)+3p_2^2M_1(\Gamma_1)+2p_2^3q_1 \\ &\quad + Y(\Gamma_2)+3p_1F(\Gamma_2)+3p_1^2M_1(\Gamma_2)+2p_1^3q_2 \\ &\quad + p_2F(\Gamma_1)+3p_2^2M_1(\Gamma_1)+6q_1p_2^3+p_1p_2^4 \\ &\quad + p_1F(\Gamma_2)+3p_1^2M_1(\Gamma_2)+6q_2p_1^3+p_2p_1^4. \end{aligned} \tag{12}$$

□

Theorem 3. *Let Γ_1 and Γ_2 be two undirected connected graphs with p_1, p_2 vertices and q_1, q_2 edges, then*

$$\begin{aligned} Y(\overline{\Gamma_1+\Gamma_2}) &= (p_1+p_2)(p_1+p_2-1)^4 - 8(q_1+q_2+p_1p_2)(p_1+p_2-1)^3 \\ &\quad + 6(p_1+p_2-1)^2\left[M_1(\Gamma_1)+M_1(\Gamma_2)+p_1p_2^2+p_2p_1^2+4q_1p_2+4q_2p_1\right] \\ &\quad - 4(p_1+p_2-1)\left[F(\Gamma_1)+F(\Gamma_2)+3p_2M_1(\Gamma_1)+3p_1M_1(\Gamma_2)+6p_2^2q_1\right. \\ &\quad \left.+6p_1^2q_2+p_1p_2^3+p_2p_1^3\right]+Y(\Gamma_1)+4p_2F(\Gamma_1)+6p_2^2M_1(\Gamma_1) \\ &\quad + 8q_1p_2^3+p_1p_2^4+Y(\Gamma_2)+4p_1F(\Gamma_2)+6p_1^2M_1(\Gamma_2)+8q_2p_1^3+p_2p_1^4. \end{aligned} \tag{13}$$

Proof. From Theorem 2 and since $M_1(\Gamma_1+\Gamma_2) = M_1(\Gamma_1) + M_1(\Gamma_2) + p_1p_2^2 + p_2p_1^2 + 4q_1p_2 + 4q_2p_1$ and $F(\Gamma_1+\Gamma_2) = F(\Gamma_1) + F(\Gamma_2) + 3p_2M_1(\Gamma_1) + 3p_1M_1(\Gamma_2) + 6p_2^2q_1 + 6p_1^2q_2 + p_1p_2^3 + p_2p_1^3$ are given in [26, 27], respectively, and applying equation (6), we get the required. □

Theorem 4. *The $Y-$ index of $(\overline{\Gamma_1\times\Gamma_2})$ is given by*

$$\begin{aligned} Y(\overline{\Gamma_1\times\Gamma_2}) &= p_1p_2(p_1p_2-1)^4 - 8(q_1p_2+p_1q_2)(p_1p_2-1)^3 \\ &\quad + 6(p_1p_2-1)^2\left[p_2M_1(\Gamma_1)+p_1M_1(\Gamma_2)+8q_1q_2\right] \\ &\quad - 4(p_1p_2-1)\left[p_2F(\Gamma_1)+p_1F(\Gamma_2)+6q_2M_1(\Gamma_1)+6q_1M_1(\Gamma_2)\right] \\ &\quad + p_2Y(\Gamma_1)+p_1Y(\Gamma_2)+8q_1F(\Gamma_2)+8q_2F(\Gamma_1)+6M_1(\Gamma_1)M_1(\Gamma_2). \end{aligned} \tag{14}$$

Proof. Since $M_1(\Gamma_1\times\Gamma_2)=p_2M_1(\Gamma_1)+p_1M_1(\Gamma_2)+8q_1q_2$, $F(\Gamma_1\times\Gamma_2)=p_2F(\Gamma_1)+p_1F(\Gamma_2)+6q_2M_1(\Gamma_1)+6q_1M_1(\Gamma_2)$, and $Y(\Gamma_1\times\Gamma_2)=p_2Y(\Gamma_1)+p_1Y(\Gamma_2)+8q_1F(\Gamma_2)+8q_2F(\Gamma_1)+6M_1(\Gamma_1)M_1(\Gamma_2)$ are given in [18, 28, 29], respectively, and applying equation (6), we get the required. □

Theorem 5. *Let Γ_1 and Γ_2 be two undirected connected graphs with p_1,p_2 vertices and q_1,q_2 edges, then*

$$\begin{aligned}Y(\overline{\Gamma_1\circ\Gamma_2})&=p_1p_2(p_1p_2-1)^4-8\left(q_1p_2^2+q_2p_1\right)(p_1p_2-1)^3\\&+6(p_1p_2-1)^2\left[p_2^3M_1(\Gamma_1)+p_1M_1(\Gamma_2)+8p_2q_2q_1\right]\\&-4(p_1p_2-1)\left[p_2^4F(\Gamma_1)+p_1F(\Gamma_2)+6p_2^2q_2M_1(\Gamma_1)+6p_2q_1M_1(\Gamma_2)\right]\\&+p_2^5Y(\Gamma_1)+p_1Y(\Gamma_2)+8p_2^3q_2F(\Gamma_1)+8p_2q_1F(\Gamma_2)+6p_2^2M_1(\Gamma_1)M_1(\Gamma_2).\end{aligned}\tag{15}$$

Proof. Since $M_1(\Gamma_1\circ\Gamma_2)=p_2^3M_1(\Gamma_1)+p_1M_1(\Gamma_2)+8p_2q_2q_1$, $F(\Gamma_1\circ G_2)=p_2^4F(\Gamma_1)+p_1F(\Gamma_2)+6p_2^2q_2M_1(\Gamma_1)+6p_2q_1M_1(\Gamma_2)$, and $Y(\Gamma_1\Gamma_2)=p_2^5Y(\Gamma_1)+p_1Y(\Gamma_2)+8p_2^3q_2F(\Gamma_1)+8p_2q_1F(\Gamma_2)+6p_2^2M_1(\Gamma_1)M_1(\Gamma_2)$ are given in [14, 18, 27], respectively, and applying equation (6), we get the required. □

Theorem 6. *The $Y-$index of $(\overline{\Gamma_1*\Gamma_2})$ is given by*

$$\begin{aligned}Y(\overline{\Gamma_1*\Gamma_2})&=p_1p_2(p_1p_2-1)^4-8(q_1p_2+p_1q_2+2q_1q_2)(p_1p_2-1)^3\\&+6(p_1p_2-1)^2[(p_2+6q_2)M_1(\Gamma_1)+8q_2q_1+(6q_1+p_1)M_1(\Gamma_2)\\&+2M_1(\Gamma_1)M_1(\Gamma_2)]-4(p_1p_2-1)[p_2F(\Gamma_1)+p_1F(\Gamma_2)+F(G_1)F(\Gamma_2)\\&+6q_2M_1(\Gamma_1)+6q_1M_1(\Gamma_2)+6q_2F(\Gamma_1)+6q_1F(\Gamma_2)\\&+3F(\Gamma_2)M_1(\Gamma_1)+3F(\Gamma_1)M_1(\Gamma_2)+6M_1(\Gamma_1)M_1(\Gamma_2)]\\&+Y(\Gamma_1)[4F(\Gamma_2)+6M_1(\Gamma_2)+8q_2+p_2]+4F(\Gamma_1)[3M_1(\Gamma_2)+2q_2]\\&+Y(\Gamma_2)[4F(\Gamma_1)+6M_1(\Gamma_1)+8q_1+p_1]+4F(\Gamma_2)[3M_1(\Gamma_1)+2q_1]\\&+Y(\Gamma_1)Y(\Gamma_2)+12F(\Gamma_1)F(\Gamma_2)+6M_1(\Gamma_1)M_1(\Gamma_2).\end{aligned}\tag{16}$$

Proof. By [27, 28, 30], respectively, we have

$$\begin{aligned}M_1(\Gamma_1*\Gamma_2)&=(p_2+6q_2)M_1(\Gamma_1)+8q_2q_1+(6q_1+p_1)M_1(\Gamma_2)+2M_1(\Gamma_1)M_1(\Gamma_2),\\F(\Gamma_1*\Gamma_2)&=p_2F(\Gamma_1)+p_1F(\Gamma_2)+F(\Gamma_1)F(\Gamma_2)+6q_2M_1(\Gamma_1)+6q_1M_1(\Gamma_2)+6q_2F(\Gamma_1)+6q_1F(\Gamma_2)+3F(\Gamma_2)M_1(\Gamma_1)\\&+3F(\Gamma_1)M_1(\Gamma_2)+6M_1(\Gamma_1)M_1(\Gamma_2),\\Y(\Gamma_1*\Gamma_2)&=Y(\Gamma_1)[4F(\Gamma_2)+6M_1(\Gamma_2)+8q_2+p_2]+4F(\Gamma_1)[3M_1(\Gamma_2)+2q_2]+Y(\Gamma_2)[4F(\Gamma_1)+6M_1(\Gamma_1)+8q_1+p_1]\\&+4F(\Gamma_2)[3M_1(\Gamma_1)+2q_1]\\&+Y(\Gamma_1)Y(\Gamma_2)+12F(\Gamma_1)F(\Gamma_2)+6M_1(\Gamma_1)M_1(\Gamma_2).\end{aligned}\tag{17}$$

Also, by applying equation (6), we get the required. □

Theorem 7. *The Y − index of $(\overline{\Gamma_1 \vee \Gamma_2})$ is given by*

$$\begin{aligned} Y(\overline{\Gamma_1 \vee \Gamma_2}) = {} & p_1p_2(p_1p_2-1)^4 - 8\big(q_1p_2^2+q_2p_1^2-2q_1q_2\big)(p_1p_2-1)^3 \\ & +6(p_1p_2-1)^2\big[\big[p_2^3-4p_2q_2\big]M_1(\Gamma_1)+\big[p_1^3-4p_1q_1\big]M_1(\Gamma_2)+8p_1p_2q_1q_2+M_1(\Gamma_1)M_1(\Gamma_2)\big] \\ & -4(p_1p_2-1)\big[p_2^4F(\Gamma_1) \\ & +p_1^4F(\Gamma_2)-F(\Gamma_1)F(\Gamma_2)+6p_1p_2^2q_2M_1(\Gamma_1)+6p_2p_1^2q_1M_1(\Gamma_2) \\ & +3p_2F(\Gamma_1)M_1(\Gamma_2)+3p_1F(\Gamma_2)M_1(\Gamma_1)-6p_2^2q_2F(\Gamma_1)-6p_1^2q_1F(\Gamma_2) \\ & -6p_1p_2M_1(\Gamma_1)M_1(\Gamma_2)\big]+p_1Y(\Gamma_2)\big[p_1^4+6p_1M_1(\Gamma_1)-8p_1^2q_1-4F(\Gamma_1)\big] \\ & +4p_1^2p_2F(\Gamma_2)[2p_1q_1-3M_1(\Gamma_1)]+p_2Y(\Gamma_1)\big[p_2^4+6p_2M_1(\Gamma_2)-8p_2^2q_2 \\ & -4F(\Gamma_2)\big]+4p_2^2p_1F(\Gamma_1)[2p_2q_2-3M_1(\Gamma_2)]+Y(\Gamma_1)Y(\Gamma_2) \\ & +12p_1p_2F(\Gamma_1)F(\Gamma_2)+6p_1^2p_2^2M_1(\Gamma_1)M_1(\Gamma_2). \end{aligned} \tag{18}$$

Proof. By [14, 27, 31], respectively, we have

$$\begin{aligned} M_1(\Gamma_1\vee\Gamma_2) &= \big[p_2^3-4p_2q_2\big]M_1(\Gamma_1)+\big[p_1^3-4p_1q_1\big]M_1(\Gamma_2)+8p_1q_2q_1q_2+M_1(\Gamma_1)M_1(\Gamma_2) \\ F(\Gamma_1\vee\Gamma_2) &= p_2^4F(\Gamma_1)+p_1^4F(\Gamma_2)-F(\Gamma_1)F(\Gamma_2)+6p_1p_2^2q_2M_1(\Gamma_1)+6p_2p_1^2q_1M_1(\Gamma_2)+3p_2F(\Gamma_1)M_1(\Gamma_2) \\ &\quad +3p_1F(\Gamma_2)M_1(\Gamma_1)-6p_2^2q_2F(\Gamma_1)-6p_1^2q_1F(\Gamma_2)-6p_1p_2M_1(\Gamma_1)M_1(\Gamma_2), \\ Y(\Gamma_1\vee\Gamma_2) &= p_1Y(\Gamma_2)\big[p_1^4+6p_1M_1(\Gamma_1)-8p_1^2q_1-4F(\Gamma_1)\big]+4p_1^2p_2F(\Gamma_2)[2p_1q_1-3M_1(\Gamma_1)] \\ &\quad +p_2Y(\Gamma_1)\big[p_2^4+6p_2M_1(\Gamma_2)-8p_2^2q_2-4F(\Gamma_2)\big]+4p_2^2p_1F(\Gamma_1)[2p_2q_2-3M_1(\Gamma_2)] \\ &\quad +Y(\Gamma_1)Y(\Gamma_2)+12p_1p_2F(\Gamma_1)F(\Gamma_2)+6p_1^2p_2^2M_1(\Gamma_1)M_1(\Gamma_2). \end{aligned} \tag{19}$$

Also, by applying equation (6) for $(\overline{\Gamma_1 \vee \Gamma_2})$, we get the required. □

Theorem 8. *The Y − index of complement $(\Gamma_1 \oplus \Gamma_2)$ is given by*

$$\begin{aligned} Y(\overline{\Gamma_1 \oplus \Gamma_2}) = {} & p_1p_2(p_1p_2-1)^4 - 8\big(q_1p_2^2+q_2p_1^2-4q_1q_2\big)(p_1p_2-1)^3 \\ & +6(p_1p_2-1)^2\big[\big[p_2^3-8p_2q_2\big]M_1(\Gamma_1)+\big[p_1^3-8p_1q_1\big]M_1(\Gamma_2) \\ & +8p_1p_2q_1q_2+4M_1(\Gamma_1)M_1(\Gamma_2)\big]-4(p_1p_2-1)\big[p_2^4F(\Gamma_1) \\ & +p_1^4F(\Gamma_2)-8F(\Gamma_1)F(\Gamma_2)+6p_1p_2^2q_2M_1(\Gamma_1)+6p_2p_1^2q_1M_1(\Gamma_2) \\ & +12p_2F(\Gamma_1)M_1(\Gamma_2)+12p_1F(\Gamma_2)M_1(\Gamma_1)-12p_2^2q_2F(\Gamma_1) \\ & -12p_1^2q_1F(\Gamma_2)-12p_1p_2M_1(\Gamma_1)M_1(\Gamma_2)\big] \\ & +p_1Y(\Gamma_2)\big[p_1^4+24p_1M_1(\Gamma_1)-16n_1^2q_1-32F(\Gamma_1)\big] \\ & +8p_1^2p_2F(\Gamma_2)[p_1q_1-3M_1(\Gamma_1)]+8p_2^2p_1F(\Gamma_1)[p_2q_2-3M_1(\Gamma_2)] \\ & +p_2Y(\Gamma_1)\big[p_2^4+24p_2M_1(\Gamma_2)-16p_2^2q_2-32F(\Gamma_2)\big] \\ & +16Y(\Gamma_1)Y(\Gamma_2)+48p_1p_2F(\Gamma_1)F(\Gamma_2)+6p_1^2p_2^2M_1(\Gamma_1)M_1(\Gamma_2). \end{aligned} \tag{20}$$

Proof. By using the same method such as in Theorem 7, we get the required. □

2.2. Y-Polynomial of Titania Nanotubes and Y-Index of Molecular Complement Titania Nanotubes. Titania nanotubes are semiconductors that have been systematically synthesized and studied carefully as potential technological materials [32–34], and some authors have calculated some of its topological indices [32–35]. In the following theorems and corollaries, we obtained the formula for $Y-$polynomial of titania nanotubes and computed the general expressions for the $Y-$index of complement structure of titania nanotubes.

Theorem 9. *Let* $\Psi = TiO_2[q,p]$ *be titania nanotubes (see Figure 2). Then,* $Y-$*polynomial of* Ψ *is given by*

$$Y(\Psi,x) = q\left[6x^{72} + (4p+2)x^{133} + 2x^{91} + (6p-2)x^{152}\right]. \tag{21}$$

Proof. Since the definition of Y-polynomial of the graph Γ is $Y(\Gamma,x) = \sum_{\mu\nu\in E(\Gamma)} x^{[\delta_\Gamma^3(\mu)+\delta_\Gamma^3(\nu)]}$, the vertex and edge partitions $V(\Psi), E(\Psi)$ of titania nanotube are given as Corollary 4.1 in [30], and the edge set of Ψ is divided into four edges, depending on the degree of the vertices as follows:

$$\begin{aligned} E_8^*(\Psi) &= \{e=\mu\nu\in E(\Psi)\colon \delta(\mu)=2, \delta(\nu)=4\},\\ E_{10}^*(\Psi) &= \{e=\mu\nu\in E(\Psi)\colon \delta(\mu)=2, \delta(\nu)=5\},\\ E_{12}^*(\Psi) &= \{e=\mu\nu\in E(\Psi)\colon \delta(\mu)=3, \delta(\nu)=4\},\\ E_{15}^*(\Psi) &= \{e=\mu\nu\in E(\Psi)\colon \delta(\mu)=3, \delta(\nu)=5\}. \end{aligned} \tag{22}$$

Therefore,

$$\begin{aligned} Y(\Psi,x) &= \sum_{\mu\nu\in E(\Psi)} x^{\left[\delta_\Psi^3(\mu)+\delta_\Psi^3(\nu)\right]} = \sum_{\mu\nu\in E_8^*(\Psi)} x^{\left[\delta_\Psi^3(\mu)+\delta_\Psi^3(\nu)\right]}\\ &\quad + \sum_{\mu\nu\in E_{10}^*(\Psi)} x^{\left[\delta_\Psi^3(\mu)+\delta_\Psi^3(\nu)\right]} + \sum_{\mu\nu\in E_{12}^*(\Psi)} x^{\left[\delta_\Psi^3(\mu)+\delta_\Psi^3(\nu)\right]} + \sum_{\mu\nu\in E_{15}^*(\Psi)} x^{\left[\delta_\Psi^3(\mu)+\delta_\Psi^3(\nu)\right]}\\ &= \left|E_8^*(\Psi)\right| x^{2^3+4^3} + \left|E_{10}^*(\Psi)\right| x^{2^3+5^3}\\ &\quad + \left|E_{12}^*(\Psi)\right| x^{3^3+4^3} + \left|E_{15}^*(\Psi)\right| x^{3^3+5^3}\\ &= 6qx^{2^3+4^3} + [4qp+2q]x^{2^3+5^3} + 2qx^{3^3+4^3} + [6qp-2q]x^{3^3+5^3}. \end{aligned} \tag{23}$$

□

Corollary 10. *The Y-index of complement* $\Psi = TiO_2[q,p]$ *nanotube is given by*

$$\begin{aligned} Y(\overline{\Psi}) &= 2q(6pq+6n-1)^3[3(p+1)(6pq+6q-1) - 8(5p+4)]\\ &\quad + 8q(6pq+6q-1)[3(6pq+6q-1)(19p+12) - 80(2p+1)]\\ &\quad + 1444pq + 576q. \end{aligned} \tag{24}$$

Proof. From [32, 36], we have $F(\Psi) = 320qp + 160q$, $M_1(\Psi) = 76qp + 48q$, and $Y(\Psi) = 1444qp + 576q$, and the collection of the cardinality of the vertex and edge sets of titania nanotubes are given as $\sum|V\Psi)| = 6qp + 6q$, $\sum|E(\Psi)| = 10qp + 8q$.

Also, by applying equation (6) for $\overline{\Psi}[q,p]$, we have

$$\begin{aligned} Y(\overline{\Psi}) &= \sum|V(\Psi|\left(\sum|V(\Psi)|-1\right)^4 - 8\sum|E(\Psi)|\left(\sum|V(\Psi)|-1\right)^3\\ &\quad + 6\left(\sum|V(\Psi)|-1\right)^2 M_1(\Psi) - 4\left(\sum|V(\Psi)|-1\right)F(\Psi) + Y(\Psi)\\ &= 2q(6pq+6q-1)^3[3(p+1)(6qp+6q-1) - 8(5p+4)]\\ &\quad + 8q(6pq+6q-1)[3(6qp+6q-1)(19p+12) - 80(2p+1)]\\ &\quad + 1444qp + 576q. \end{aligned} \tag{25}$$

□

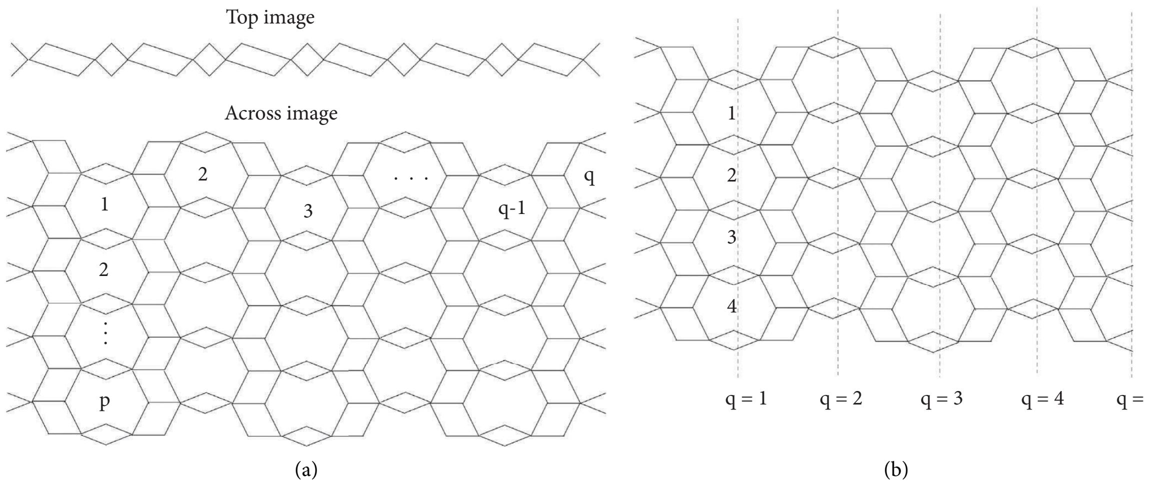


FIGURE 2: The molecular graph of TiO_2 $[q, p]$ nanotube.

2.3. Y-Index of $HAC_5C_7[q, p]$ Nanotube $(q, p \geq 1)$. In this subsection, we present some formulae for the $Y-$ index and $-$coindex of the $HAC_5C_7[m, n]$ nanotubes and its molecular complement graph. Moreover, we apply $Y-$ *polynomial* on the line graphs of the $HAC_5C_7[m, n]$ nanotubes.

Theorem 11. *Let $\Theta = HAC_5C_7[q, p]$ nanotube and the $Y-$ index of Θ (Figure 3) is given by*

$$Y(\Theta) = 17496\text{qp} - 5970q. \tag{26}$$

Proof. The vertex and edge partitions $V(\Theta)$ and $E(\Theta)$ of Θ are given in Tables 1 and 2, respectively.

The edge set of $\Theta = HAC_5C_7[q, p]$ for the sum degree on the neighbors of each vertex can be divided into six separate edges as follows:

$$\begin{aligned}
E_1(\Theta) &= \{\mu\nu \in E(\Theta)\colon \delta(\mu) = 6, \delta(\nu) = 7\},\\
E_2(\Theta) &= \{\mu\nu \in E(\Theta)\colon \delta(\mu) = 6, \delta(\nu) = 8\},\\
E_3(\Theta) &= \{\mu\nu \in E(\Theta)\colon \delta(\mu) = 7, \delta(\nu) = 9\},\\
E_4(\Theta) &= \{\mu\nu \in E(\Theta)\colon \delta(\mu) = 8, \delta(\nu) = 8\},\\
E_5(\Theta) &= \{\mu\nu \in E(\Theta)\colon \delta(\mu) = 8, \delta(\nu) = 9\},\\
E_6(\Theta) &= \{\mu\nu \in E(\Theta)\colon \delta(\mu) = 9, \delta(\nu) = 9\}.
\end{aligned} \tag{27}$$

Therefore, by using the definition of the $Y-$ index, we have

$$\begin{aligned}
Y(\Theta) &= \sum_{\mu\nu\in E(\Theta)} \left[\delta_\Theta^3(\mu) + \delta_\Theta^3(\nu)\right] = \sum_{\mu\nu\in E_{i=1}(\Theta)}^{6} \left[\delta_\Theta^3(\mu) + \delta_\Theta^3(\nu)\right]\\
&= 559|E_1(\Theta)| + 728|E_2(\Theta)| + 1072|E_3(\Theta)| + 1024|E_4(\Theta)|\\
&\quad + 1241|E_5(\Theta)| + 1458|E_6(\Theta)|.
\end{aligned} \tag{28}$$

□

Corollary 12. *The $Y-$ polynomial of $\Theta = HAC_5C_7[q, p]$ nanotube (Figure 3) is given by*

$$Y(\Theta, x) = q\left[2x^{559} + 2x^{728} + x^{1072} + x^{1024} + 2x^{1241} + [12p - 9]x^{1458}\right]. \tag{29}$$

Proof. By the definition of the $(Y-$ index$)$ and Theorem 11, we have

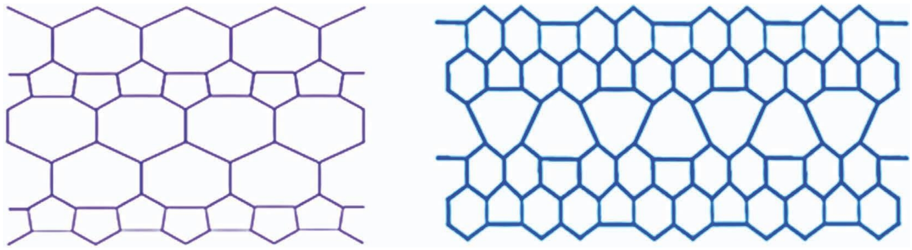


FIGURE 3: The molecular structures of $\Theta = HAC_5C_7[q, p]$ nanotube and $\Phi = HAC_5C_6C_7[4,2]$ nanotube, respectively.

TABLE 1: The vertex partition of $\Theta = HAC_5C_7[q, p]$ nanotubes.

Vertex partitions	Cardinality
V_2	$2q+2$
V_3	$8qp-q-2$

TABLE 2: The edge partition of $\Theta = HAC_5C_7[q, p]$ nanotubes.

Edge partitions	Cardinality
E_1	$2q$
E_2	$2q$
E_3	q
E_4	q
E_5	$2q$
E_6	$12qp-9q$

$$\begin{aligned} Y(\Theta, x) &= \sum_{\mu\nu\in E(\Theta)} x^{\left[\delta_\Theta^3(\mu)+\delta_\Theta^3(\nu)\right]} = \sum_{\mu\nu\in E_{i=1}(\Theta)}^{6} x^{\left[\delta_\Theta^3(\mu)+\delta_\Theta^3(\nu)\right]} \\ &= \left|E_1(\Theta)\right|x^{559} + \left|E_2(\Theta)\right|x^{728} + \left|E_3(\Theta)\right|x^{1072} + \left|E_4(\Theta)\right|x^{1024} \\ &\quad + \left|E_5(\Theta)\right|x^{1241} + \left|E_6(\Theta)\right|x^{1458}. \end{aligned} \tag{30}$$

□

Theorem 13. *The forgotten index of $\Theta = HAC_5C_7[q, p]$ nanotube (Figure 3) is given by*

$$F(\Theta) = 1944qp - 640q. \tag{31}$$

Proof. Using the definition of the $F-$index, we get

$$\begin{aligned} F(\Theta) &= \sum_{\mu\nu\in E(\Theta)} \left[\delta_\Theta^2(\mu) + \delta_\Theta^2(\nu)\right] = \sum_{\mu\nu\in E_{i=1}(\Theta)}^{6} \left[\delta_\Theta^2(\mu) + \delta_\Theta^2(\nu)\right] \\ &= 85\left|E_1(\Theta)\right| + 100\left|E_2(\Theta)\right| + 130\left|E_3(\Theta)\right| + 128\left|E_4(\Theta)\right| \\ &\quad + 145\left|E_5(\Theta)\right| + 162\left|E_6(\Theta)\right|. \end{aligned} \tag{32}$$

□

Theorem 14 (see [37]). *The 1st & 2nd Zagreb indices and hyper-Zagreb index of $\Theta = HAC_5C_7[q, p]$ nanotube are given by*

$$\begin{aligned} M_1(\Theta) &= 216\mathrm{qp} - 42q.\\ M_2(\Theta) &= 972\mathrm{qp} - 278q.\\ \mathrm{HM}(\Theta) &= 3888\mathrm{qp} - 1092q. \end{aligned} \tag{33}$$

Corollary 15. *The $F-$polynomial of $\Theta = HAC_5C_7[q,p]$ nanotube (Figure 3) is given by*

$$F(\Theta, x) = q\left[2x^{85} + 2x^{100} + x^{130} + x^{128} + 2x^{145} + [12p - 9]x^{162}\right]. \tag{34}$$

Proof. By the definition of the $(F-\text{index})$ and Theorem 13, we have

$$\begin{aligned} F(\Theta, x) &= \sum_{\mu\nu\in E(\Theta)} x^{\left[\delta_\Theta^2(\mu)+\delta_\Theta^2(\nu)\right]} = \sum_{\mu\nu\in E_{i=1}(\Theta)}^{6} x^{\left[\delta_\Theta^2(\mu)+\delta_\Theta^2(\nu)\right]}\\ &= |E_1(\Theta)|x^{6^2+7^2} + |E_2(\Theta)|x^{6^2+8^2} + |E_3(\Theta)|x^{7^2+9^2} + |E_4(\Theta)|x^{8^2+8^2}\\ &\quad + |E_5(\Theta)|x^{8^2+9^2} + |E_6(\Theta)|x^{9^2+9^2}. \end{aligned} \tag{35}$$

□

Corollary 16. *The $Y-$index of the complement $\Theta = HAC_5C_7[q,p]$ nanotube (Figure 3) is given by*

$$\begin{aligned} Y(\overline{\Theta}) &= [8\mathrm{qp} + q](8\mathrm{qp} + q - 1)^4 - 8[12\mathrm{qp} - q](8\mathrm{qp} + q - 1)^3\\ &\quad + 6(8\mathrm{qp} + q - 1)^2[216\mathrm{qp} - 42q] - 4(8\mathrm{qp} + q - 1)[1944\mathrm{qp} - 640q] + 17496\mathrm{qp} - 5970q. \end{aligned} \tag{36}$$

Proof. From Theorems 11 and 13, $F(\Theta) = 1944\mathrm{qp} - 640q$, $M_1(\Theta) = 216\mathrm{qp} - 42q$, and $Y(\Theta) = 17496\mathrm{qp} - 5970q$; moreover, the collection of the cardinality of the vertex and edge sets of $\Theta = HAC_5C_7[q,p]$ nanotube are

$$\begin{aligned} \sum|V(\Theta)| &= 8\mathrm{qp} + q,\\ \sum|E(\Theta)| &= 12\mathrm{qp} - q. \end{aligned} \tag{37}$$

Also, by applying equation (6) for $\overline{\Theta}[q,p]$, we obtain

$$\begin{aligned} Y(\overline{\Theta}) &= \sum|V(\Theta)|\left(\sum|V(\Theta)| - 1\right)^4 - 8\sum|E(\Theta)|\left(\sum|V(\Theta)| - 1\right)^3\\ &\quad + 6\left(\sum|V(\Theta)| - 1\right)^2 M_1(\Theta) - 4\left(\sum|V(\Theta)| - 1\right)F(\Theta) + Y(\Theta)\\ &= [8\mathrm{qp} + q](8\mathrm{qp} + q - 1)^4 - 8[12\mathrm{qp} - q](8\mathrm{qp} + q - 1)^3\\ &\quad + 6(8\mathrm{qp} + q - 1)^2 M_1(\Theta) - 4(8\mathrm{qp} + q - 1)F(\Theta) + Y(\Theta). \end{aligned} \tag{38}$$

□

Theorem 17. *The $Y-$coindex of $\Theta = HAC_5C_7[q,p]$ nanotube (Figure 3) is given by*

$$\overline{Y}(\Theta) = (8\mathrm{qp} + q)[1944\mathrm{qp} - 640q] - 19440\mathrm{qp} + 6610q. \tag{39}$$

Proof. Using Theorems 11 and 13 and applying equation (7), we get the required. □

2.4. Y-Index of $HAC_5C_6C_7[q,p]$ Nanotube $(q, p \geq 1)$. In this subsection, we compute the $Y-$index and $-$coindex of the $HAC_5C_6C_7[q,p]$ nanotubes and its molecular complement graph. Moreover, we apply $Y-$polynomial on the line graphs of the $HAC_5C_6C_7[q,p]$ nanotubes.

Theorem 18. *Let ($\Phi = HAC_5C_6C_7[q,p]$ nanotube), then the $Y-$index of Φ (Figure 3) is given by*

$$Y(\Phi) = 34992\mathrm{qp} - 12374q. \tag{40}$$

Proof. The vertex and edge partitions $V(\Phi)$ and $E(\Phi)$ of Φ are given in Tables 3 and 4, respectively.

The edge set of $\Phi = HAC_5C_6C_7[q,p]$ can be divided into six disjoint edge sets as follows:

$$\begin{aligned}
E_1(\Phi) &= \{e = \mu\nu \in E(\Phi)\colon \delta(\mu) = 6, \delta(\nu) = 7\},\\
E_2(\Phi) &= \{e = \mu\nu \in E(\Phi)\colon \delta(\mu) = 6, \delta(\nu) = 8\},\\
E_3(\Phi) &= \{e = \mu\nu \in E(\Phi)\colon \delta(\mu) = 7, \delta(\nu) = 8\},\\
E_4(\Phi) &= \{e = \mu\nu \in E(\Phi)\colon \delta(\mu) = 8, \delta(\nu) = 8\},\\
E_5(\Phi) &= \{e = \mu\nu \in E(\Phi)\colon \delta(\mu) = 8, \delta(\nu) = 9\},\\
E_6(\Phi) &= \{e = \mu\nu \in E(\Phi)\colon \delta(\mu) = 9, \delta(\nu) = 9\}.
\end{aligned} \tag{41}$$

Therefore, by using the definition of the $Y-$ index, we have

$$\begin{aligned}
Y(\Phi) &= \sum_{\mu\nu\in E(\Phi)} \left[\delta_\Phi^3(\mu) + \delta_\Phi^3(\nu)\right] = \sum_{\mu\nu\in E_{i=1}(\Phi)}^{6} \left[\delta_\Phi^3(\mu) + \delta_\Phi^3(\nu)\right]\\
&= 559|E_1(\Phi)| + 728|E_2(\Phi)| + 855|E_3(\Phi)| + 1024|E_4(\Phi)|\\
&\quad + 1241|E_5(\Phi)| + 1458|E_6(\Phi)|.
\end{aligned} \tag{42}$$

□

Corollary 19. *The $Y-$ polynomial of $\Phi = HAC_5C_6C_7[q,p]$ nanotube (Figure 3) is given by*

$$\begin{aligned}
Y(\Phi, x) &= 2q\left[2x^{559} + 2x^{728} + x^{855} + x^{1024} + 2x^{1241}\right.\\
&\quad \left. + [12p - 9]x^{1458}\right].
\end{aligned} \tag{43}$$

Proof. By the definition of the ($Y-$ index) and Theorem 18, we have

$$\begin{aligned}
Y(\Phi, x) &= \sum_{\mu\nu\in E(\Phi)} x^{\left[\delta_\Phi^3(\mu)+\delta_\Phi^3(\nu)\right]}\\
&= \sum_{\mu\nu\in E_{i=1}(\Phi)}^{6} x^{\left[\delta_\Phi^3(\mu)+\delta_\Phi^3(\nu)\right]}\\
&= |E_1(\Phi)|x^{559} + |E_2(\Phi)|x^{728} + |E_3(\Phi)|x^{855} + |E_4(\Phi)|x^{1024}\\
&\quad + |E_5(\Phi)|x^{1241} + |E_6(\Phi)|x^{1458}.
\end{aligned} \tag{44}$$

□

Theorem 20. *Let $\Phi = HAC_5C_6C_7[q,p]$ nanotube, then the forgotten index of Φ (Figure 3) is given by*

$$F(\Phi) = 3888\text{qp} - 2320q. \tag{45}$$

Proof. By using the definition of the $F-$ index, we get

$$\begin{aligned}
F(\Phi) &= \sum_{\mu\nu\in E(\Phi)} \left[\delta_\Phi^2(\mu) + \delta_\Phi^2(\nu)\right] = \sum_{\mu\nu\in E_{i=1}(\Phi)}^{6} \left[\delta_\Phi^2(\mu) + \delta_\Phi^2(\nu)\right]\\
&= 430|E_1(\Phi)| + 400|E_2(\Phi)| + 226|E_3(\Phi)| + 256|E_4(\Phi)|\\
&\quad + 580|E_5(\Phi)| + 162|E_6(\Phi)|.
\end{aligned} \tag{46}$$

□

Theorem 21 (see [37]). *The 1st and 2nd Zagreb indices and hyper-Zagreb index of $\Phi = HAC_5C_6C_7[q,p]$ nanotube are given by*

Table 3: The vertex partition of $\Phi = HAC_5C_6C_7[q, p]$ nanotubes.

Vertex partitions	Cardinality
V_2	$2q + 2$
V_3	$8qp - q - 2$

Table 4: The edge partition of $\Phi = HAC_5C_6C_7[q, p]$ nanotubes.

Edge partitions	Cardinality
E_1	$4q$
E_2	$4q$
E_3	$2q$
E_4	$2q$
E_5	$4q$
E_6	$24qp - 18q$

$$\begin{aligned} M_1(\Phi) &= 432qp - 68q. \\ M_2(\Phi) &= 1944qp - 570q. \\ HM(\Phi) &= 7776qp - 2254q. \end{aligned} \tag{47}$$

Corollary 22. *The $F-$polynomial of $\Phi = HAC_5C_6C_7[q, p]$ nanotube (Figure 3) is given by*

$$\begin{aligned} F(\Phi, x) = q\big[&4x^{85} + 4x^{100} + 2x^{113} + 2x^{128} + 4x^{145} \\ &+ [24p - 18]x^{162}\big]. \end{aligned} \tag{48}$$

Proof. By the definition of the $(F-\text{index})$ and Theorem 20, we obtain

$$\begin{aligned} F(\Phi, x) &= \sum_{\mu\nu\in E(\Phi)} x^{[\delta_\Phi^2(\mu)+\delta_\Phi^2(\nu)]} = \sum_{\mu\nu\in E_{i=1}(\Phi)}^{6} x^{[\delta_\Phi^2(\mu)+\delta_\Phi^2(\nu)]} \\ &= |E_1(\Phi)|x^{6^2+7^2} + |E_2(\Phi)|x^{6^2+8^2} + |E_3(\Phi)|x^{7^2+8^2} + |E_4(\Phi)|x^{8^2+8^2} \\ &\quad + |E_5(\Phi)|x^{8^2+9^2} + |E_6(\Phi)|x^{9^2+9^2}. \end{aligned} \tag{49}$$

□

Corollary 23. *The $Y-$index of the complement $\Phi = HAC_5C_6C_7[q, p]$ nanotube (Figure 3) is given by*

$$\begin{aligned} Y(\overline{\Theta}) &= [8qp + q](8qp + q - 1)^4 - 8[12qp - q](8qp + q - 1)^3 \\ &\quad + 6(8qp + q - 1)^2 M_1(\Theta) - 4(8qp + q - 1)F(\Phi) + Y(\Phi). \end{aligned} \tag{50}$$

Proof. From Theorems 18 and 20, there are $F(\Phi) = 3888qp - 2320q$, $M_1(\Phi) = 432qp - 68q$, and $Y(\Phi) = 34992qp - 12374q$; furthermore, the collections of the cardinality of the vertex and edge sets of $\Phi = HAC_5C_6C_7[q, p]$ nanotube are

$$\begin{aligned} \sum |V\Phi)| &= 8qp + q, \\ \sum |E(\Phi)| &= 24qp - 2q. \end{aligned} \tag{51}$$

Also, by applying equation (6) for $\overline{\Phi}[q, p]$, we have

$$\begin{aligned} Y(\overline{\Phi}) &= \sum |V(\Phi|\big(\sum |V(\Phi)| - 1\big)^4 - 8\sum|E(\Phi)|\big(\sum |V(\Phi)| - 1\big)^3 \\ &\quad + 6\big(\sum |V(\Phi)| - 1\big)^2 M_1(\Phi) - 4\big(\sum |V(\Phi)| - 1\big)F(\Phi) + Y(\Phi) \\ &= [8qp + q](8qp + q - 1)^4 - 8[12qp - q](8qp + q - 1)^3 \\ &\quad + 6(8qp + q - 1)^2 M_1(\Theta) - 4(8qp + q - 1)F(\Phi) + Y(\Phi). \end{aligned} \tag{52}$$

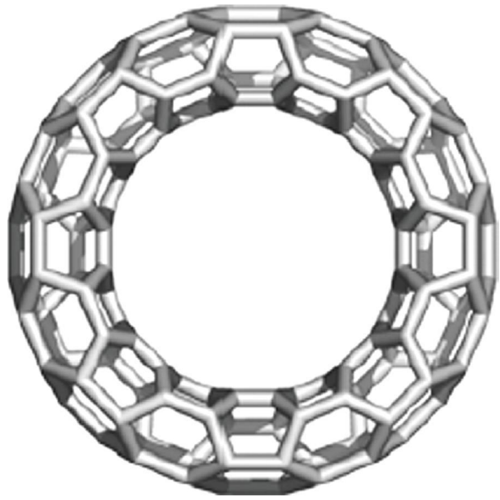


Figure 4: The molecular structure of a nanotorus.

Theorem 24. *The $Y-$coindex of $\Theta = HAC_5C_7[q,p]$ nanotube (Figure 3) is given by*

$$\overline{Y}(\Theta) = (8qp + q)[1944qp - 640q] - 19440qp + 6610q. \tag{53}$$

Proof. Using Theorems 18 and 20 and applying equation (7), we get the required. □

Corollary 25. *Assume that $T = T[p,q]$ is the molecular structure of a nanotorus (see Figure 4), then the $Y-$inde x of complement q-multiwalled nanotorus is given by*

(a) $Y(\overline{T}[p,q]) = pq[(pq-1)^3(pq-13) + 54(pq-1)(pq-3) + 81]$.

(b) $Y(\overline{P_n \times T}) = pq[(npq-1)^3(n^2pq - 21n + 8) + 2(npq-1)(75n^2pq - 54npq - 325n + 298) + 625n - 738]$.

Proof. Proving item (a) by applying equation (6) for $\overline{T}[p,q]$ and since $M_1(T) = 9pq$, $F(T) = 27pq$, $Y(T[p,q]) = 81pq$, $Y(P_n \times T) = pq(625n - 738)$ are given in [29, 38, 39], respectively, then

$$\begin{aligned} Y(\overline{T}[p,q]) &= |V(T)|(|V(T)|-1)^4 - 8|E(T)|(|V(T)|-1)^3 + 6(|V(T)|-1)^2 M_1(T) - 4(|V(T)|-1)F(T) + Y(T) \\ &= pq(pq-1)^4 - 8\frac{3}{2}pq(pq-1)^3 + 54pq(pq-1)^2 - 108pq(pq-1) + 81pq. \end{aligned} \tag{54}$$

Proving item (b) by definition of Cartesian product, we have $|E(P_n \times T)| = pq(5/2n - 1)$,$|V(P_n \times T)|= npq$ and $M_1(P_n \times T) = pq(25n - 18)$, $F(P_n \times T) = pq(125n - 122)$, and $Y(P_n \times T) = pq(625n - 738)$ are given in [24, 38, 39], respectively, and applying Theorem 4, we get the required.

2.5. Numerical and Graphical Representation. In this subsection, using MATLAB (R2022b), the numerical values of the 1st and 2nd Zagreb indices, F-index, hyper-Zagreb index, and Y-index of $HAC_5C_7[q,p]$ and $HAC_5C_6C_7[q,p]$ nanotubes have been computed. The numerical representation is depicted in Tables 5 and 6. In Table 5, data analysis of some indices' values of $HAC_5C_7[q,p]$ nanotubes are presented and formulae are reported in Theorems 11, 13, and 14 for the $HAC_5C_7[q,p]$ nanotubes. In Table 6, some indices' values of $HAC_5C_6C_7[q,p]$ nanotubes are presented and formulae are reported in Theorems 18, 20, and 21 for $HAC_5C_6C_7[q,p]$ nanotubes. In both tables, it shows that values of 1st and 2nd Zagreb indices, forgotten, hyper-Zagreb, and Yemen indices are in increasing order as the values of q, p increase.

The graphical representations are shown in Figures 5–9. In Figures 7–9, numerical comparison of Y-polynomial of titania nanotubes and $HAC_5C_7[q,p]$ and $HAC_5C_6C_7[q,p]$ nanotubes are presented. In Figures 5 and 6, a comparison of values of some widely known topological indices is presented. We can easily see that ($\forall q,p \in \mathbb{N}$), the 1st and 2nd Zagreb indices, F-index, hyper-Zagreb index, and Y-index of $HAC_5C_7[q,p]$ and $HAC_5C_6C_7[q,p]$ nanotubes are in increasing order as the values of q, p are increasing. However, the 1st and 2nd Zagreb indices have the least prediction potentials with respect to the dimension, while the hyper-Zagreb index and Y-index increase quickly as a function of dimensions.

Table 5: Data analysis of Zagreb indices, $F-$index, hyper-Zagreb index HM, and $Y-$index of $\Theta = HAC_5C_7[q,p]$ nanotube.

q,p	$M_1(\Theta)$	$F(\Theta)$	$M_2(\Theta)$	$HM(\Theta)$	$Y(\Theta)$
1,1	174	694	1304	2796	11526
2,2	780	3332	6496	13368	58044
3,3	1818	7914	15576	31716	139554
4,4	3288	14440	28544	57840	256056
5,5	5190	22910	45400	91740	407550
6,6	7524	33324	66144	133416	594036
7,7	10290	45682	90776	182868	815514
8,8	13488	59984	119296	240096	1071984
9,9	17118	76230	151704	305100	1363446
10,10	21180	94420	188000	377880	1689900

Table 6: Data analysis of Zagreb indices, $F-$index, hyper-Zagreb index HM, and $Y-$index of $\Phi = HAC_5C_6C_7[q,p]$ nanotube.

q,p	$M_1(\Phi)$	$F(\Phi)$	$M_2(\Phi)$	$HM(\Phi)$	$Y(\Theta)$
1,1	364	1374	1568	5522	22618
2,2	1592	6636	10912	26596	115220
3,3	3684	15786	28032	63222	277806
4,4	6640	28824	52928	115400	510376
5,5	10460	45750	85600	183130	812930
6,6	15144	66564	126048	266412	1185468
7,7	20692	91266	174272	365246	1627990
8,8	27104	119856	230272	479632	2140496
9,9	34380	152334	294048	609570	2722986
10,10	42520	188700	365600	755060	3375460

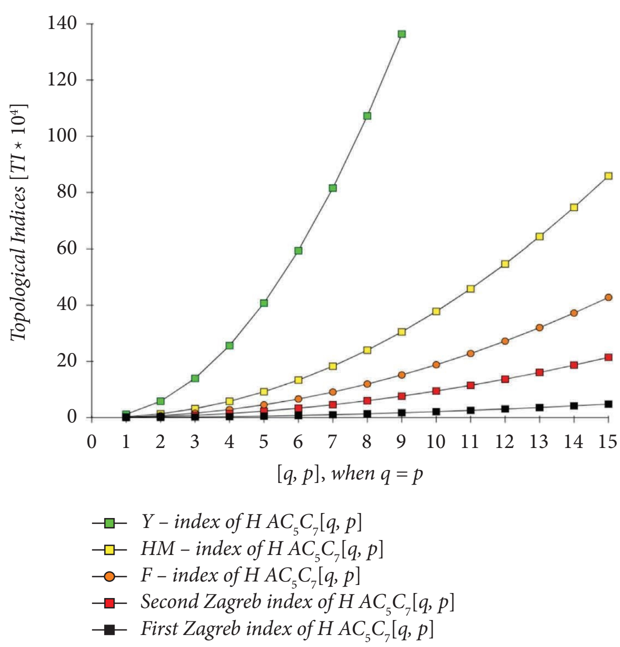


Figure 5: Comparison of 1st and 2nd Zagreb indices, F-index, hyper-Zagreb index, and Y-index of $HAC_5C_7[q,p]$ nanotube.

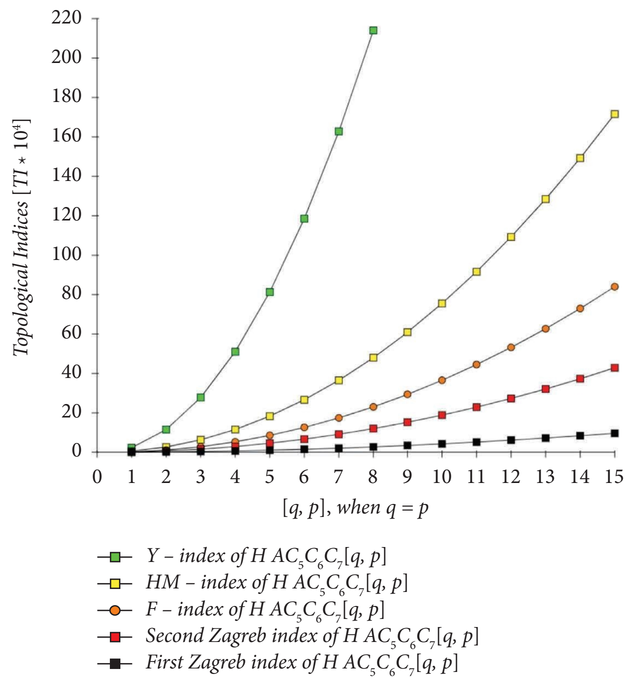


Figure 6: Comparison of 1st and 2nd Zagreb indices, F-index, hyper-Zagreb index, and Y-index of $HAC_5C_6C_7[q, p]$ nanotube.

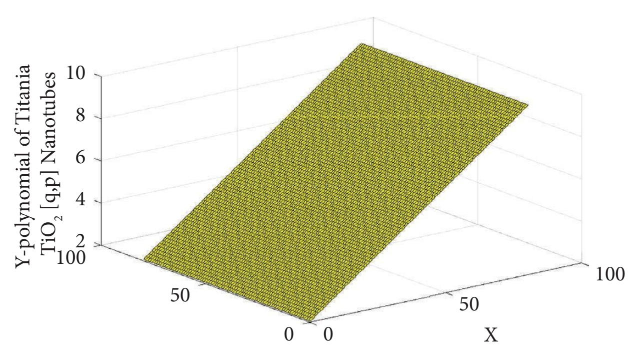


Figure 7: Y-polynomial of TiO_2.

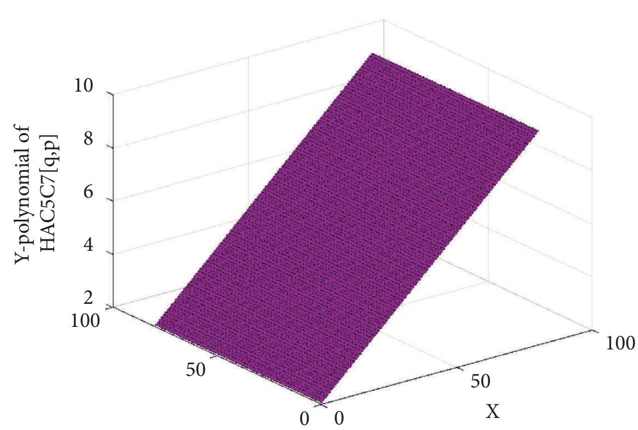


Figure 8: Y-polynomial of $HAC_5C_7[q, p]$.

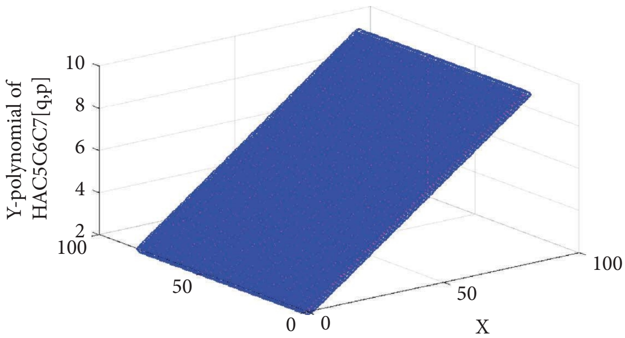


Figure 9: Y-polynomial of $HAC_5C_6C_7[q, p]$.

3. Conclusions

In light of our analysis of structures and mathematical derivations, this paper has uncovered Y-index formulae for various graph and complement graph operations. These operations include tensor and Cartesian and strong products, join, composition, disjunction, and symmetric difference of two graphs. Moreover, we have computed the Y-polynomial of titania nanotubes and the Y-index of the molecular complement graph of titania nanotubes and nanotorus. Furthermore, we have investigated the Y-index, Y-polynomial, F-index, F-polynomial, and Y-coindex formulae of $HAC_5C_7[q, p]$ and $HAC_5C_6C_7[q, p]$ nanotubes and their molecular complement graphs. To provide further insight, we have presented numerical comparisons of our computed results and illustrated corresponding graphical behavior through figures. While this research has provided valuable contributions to the field, much work remains to be done. As such, we have outlined several potential directions for future research, including the eigenvalue-based, matching-based, and mixed-based indices of nanotubes and nanotorus.

Data Availability

The data used to support the findings of this study are included within the manuscript.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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