

## Y-INDEX AND S-INDEX BASED NEW TOPOLOGICAL INDICES OF TITANIA NANOTUBES IN GRAPH

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**ABSTRACT.** Topological index is a numerical descriptor of a molecule; it is found that there is strong correlation between the properties of chemical compounds and their molecular structure based on a specific topological feature of the corresponding molecular graph. A topological index can be thought of as the conversion of a chemical structure into a real number. Titania nanotubes are a well-known semiconductor with a wide range of technological applications including biomedical devices, dye-sensitized solar cells, and so on. In this study, we introduce various types of topological indices based on *Y*-index and *S*-index of molecular graphs. Exact expressions for various topological indices of Titania (*TiO<sub>2</sub>*) nanotubes are represented.

**Keywords:** Zagreb, *Y*-index, *S*-index, Titania Nanotubes

**AMS Subject Classification:** 05C07, 05C92

### 1. INTRODUCTION

Topological and graph invariants based on distances between graph vertices are widely used for characterizing molecular graphs, establishing relationships between structural and property properties of molecules, predicting biological activities of chemical compounds, and developing chemical applications. There are several types of topological indices, including distance-based topological indices, degree-based topological indices, and counting-related polynomials. Graph theory has given chemists an interesting tool called topological indices. Molecules and molecular compounds are frequently represented by molecular graphs. A molecular graph is a graph-theoretic representation of a chemical compound's structural formula, with vertices representing atoms and edges representing chemical bonds.

Topological indices have the significance of being able to be used directly as simple numerical descriptors in comparison with physical, chemical, or biological parameters of molecules in Quantitative Structure Property Relationships (QSPR) and Quantitative Structure Activity Relationships (QSAR). In medicinal chemistry and bioinformatics, the current trend

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of numerical coding of chemical structures with topological indices or topological coindices has been quite successful.

Titania nanotubes have been synthesised systematically over the last 10-15 years using various methods and have been thoroughly studied as potential technological materials. Because the mechanism of  $TiO_2$  nanotube growth is still unknown, comprehensive theoretical studies are gaining traction.

Let's consider simple connected graph,  $P$ , each with disjoint vertex and edge sets. The degree of a vertex  $v$  is the number of edges incident on the vertex  $v$  and is expressed as  $d_P(v) = \psi_P(v)$  for every  $v \in V(P)$ .

In 1972, I. Gutman and N. Trinajstic defined the first and second Zagreb indices of a graph as [6]:

$$M_1(P) = \sum_{v \in V(P)} [\psi_P(v)^2] = \sum_{uv \in E(P)} [\psi_P(u) + \psi_P(v)]$$

$$M_2(P) = \sum_{uv \in E(P)} [\psi_P(u)\psi_P(v)]$$

In 2015, B. Furtula and I. Gutman proposed the  $F$ -index, which is defined as [5]:

$$F(P) = \sum_{v \in V(P)} [\psi_P(v)^3] = \sum_{uv \in E(P)} [\psi_P(u)^2 + \psi_P(v)^2]$$

In 2020, Abdu Alameri and Noman AI-Naggar introduced the  $Y$ -index, which is defined as [1]:

$$Y(P) = \sum_{v \in V(P)} [\psi_P(v)^4] = \sum_{uv \in E(P)} [\psi_P(u)^3 + \psi_P(v)^3]$$

In 2021, S. Nagarajan and G. Kayalvizhi and G. Priyadharsini defined the  $S$ -index as [21]:

$$S(P) = \sum_{v \in V(P)} [\psi_P(v)^5] = \sum_{uv \in E(P)} [\psi_P(u)^4 + \psi_P(v)^4]$$

In [2018,2019, 2020] V. R. Kulli [15,11,12,17,13] determined the Titania Nanotubes ( $TiO_2$ ) for Multiplicative Minus F-indices, Minus indices, Minus F-indices, Reduced indices, Sigma indices, connectivity indices, Reciprocal and their polynomials. Mehdi Rezaei and Wei Gao [20] explained the hyper Zagreb index and M-polynomial of ( $TiO_2$ ) in [2017]. A. Subhashini and J. Baskar [23] determined the topological indices based on vertex degree for ( $TiO_2$ ) in [2018]. In 2015 Malik M and Imran M [19] defined the ( $TiO_2$ ) for multiplicative Zagreb indices of graph. N. De [3] found some topological properties of the titania nanotube in [2016]. In [2015] Furtula B and Gutman I [5] proposed the F-index of a graph and V. R. Kulli [16], defined a second F-index [2019]. In [2] M. Albertson introduced the minus indices [1997]. The indices, minus indices, Reduced, Sigma and Modified indices, multiplicative indices based on Y-index and S-index of Titania ( $TiO_2$ ) nanotubes are determined in this paper.

## 2. NEW TOPOLOGICAL INDICES

The  $Y$ -index is critical for providing medical information about new drugs without conducting a chemical experiment. The  $S$ -index and the new indices listed below are important graph invariants in topological indices. In the following, we introduce a few topological indices which are extended versions of multiplicative indices, minus indices, reduced indices, sigma and Modified indices based on  $Y$ -index and  $S$ -index and find the

value of these indices for titania nanotubes. The Modified  $Y$ -index and Modified  $S$ -index of a graphs are defined as:

$$MY(P) = \sum_{v \in V(P)} \frac{1}{[\psi_P(v)^4]}$$

$$MS(P) = \sum_{v \in V(P)} \frac{1}{[\psi_P(v)^5]}$$

The Minus  $Y$ -index and Minus  $S$ -index of a graph is defined by:

$$MiY(P) = \sum_{uv \in E(P)} [|\psi_P(u)^3 - \psi_P(v)^3|]$$

$$MiS(P) = \sum_{uv \in E(P)} [|\psi_P(u)^4 - \psi_P(v)^4|]$$

The Sigma  $Y$ -index and Sigma  $S$ -index of a graph is defined by:

$$\sigma Y(P) = \sum_{uv \in E(P)} [\psi_P(u)^3 - \psi_P(v)^3]^2$$

$$\sigma S(P) = \sum_{uv \in E(P)} [\psi_P(u)^4 - \psi_P(v)^4]^2$$

The Modified Minus  $Y$ -index and Modified Minus  $S$ -index of a graph is defined by:

$$MMY(P) = \sum_{uv \in E(P)} \frac{1}{|\psi_P(u)^3 - \psi_P(v)^3|}$$

$$MMS(P) = \sum_{uv \in E(P)} \frac{1}{|\psi_P(u)^4 - \psi_P(v)^4|}$$

The Reduced  $Y$ -index and Reduced  $S$ -index of a graph is defined as:

$$ReY(P) = \sum_{v \in V(P)} [\psi_P(v) - 1]^4$$

$$ReS(P) = \sum_{v \in V(P)} [\psi_P(v) - 1]^5$$

The Reduced Modified  $Y$ -index and Reduced Modified  $S$ -index of a graph is defined as:

$$ReMY(P) = \sum_{v \in V(P)} \frac{1}{[\psi_P(v) - 1]^4}$$

$$ReMS(P) = \sum_{v \in V(P)} \frac{1}{[\psi_P(v) - 1]^5}$$

The Multiplicative  $Y$ -index and Multiplicative  $S$ -index of a graph is defined as:

$$\prod_Y(P) = \prod_{v \in V(P)} [\psi_P(v)^4]$$

$$\prod_S(P) = \prod_{v \in V(P)} [\psi_P(v)^5]$$

The Multiplicative Sigma  $Y$ -index and Multiplicative Sigma  $S$ -index of a graph is defined as:

$$\begin{aligned}\sigma_Y \prod(P) &= \prod_{uv \in E(P)} [\psi_P(u)^3 - \psi_P(v)^3]^2 \\ \sigma_S \prod(P) &= \prod_{uv \in E(P)} [\psi_P(u)^4 - \psi_P(v)^4]^2\end{aligned}$$

The Multiplicative Minus  $Y$ -index and Multiplicative Minus  $S$ -index of a graph is defined as:

$$\begin{aligned}M_Y \prod(P) &= \prod_{uv \in E(P)} [|\psi_P(u)^3 - \psi_P(v)^3|] \\ M_S \prod(P) &= \prod_{uv \in E(P)} [|\psi_P(u)^4 - \psi_P(v)^4|]\end{aligned}$$

The Multiplicative Modified Minus  $Y$ -index and Multiplicative Modified Minus  $S$ -index of a graph is defined as:

$$\begin{aligned}MM_Y \prod(P) &= \prod_{uv \in E(P)} \frac{1}{|\psi_P(u)^3 - \psi_P(v)^3|} \\ MM_S \prod(P) &= \prod_{uv \in E(P)} \frac{1}{|\psi_P(u)^4 - \psi_P(v)^4|}\end{aligned}$$

The Multiplicative Reduced  $Y$ -index and Multiplicative Reduced  $S$ -index of a graph is defined as:

$$\begin{aligned}Re_Y \prod(P) &= \prod_{v \in V(P)} [\psi_P(v) - 1]^4 \\ Re_S \prod(P) &= \prod_{v \in V(P)} [\psi_P(v) - 1]^5\end{aligned}$$

The Multiplicative Reduced Modified  $Y$ -index and Multiplicative Reduced Modified  $S$ -index of a graph is defined as:

$$\begin{aligned}ReM_Y \prod(P) &= \prod_{v \in V(P)} \frac{1}{[\psi_P(v) - 1]^4} \\ ReM_S \prod(P) &= \prod_{v \in V(P)} \frac{1}{[\psi_P(v) - 1]^5}\end{aligned}$$

### 3. TITANIA ( $TiO_2$ ) NANOTUBES

The graph of titania nanotube is depicted in Figure 1, where  $g$  denotes the number of octagons in a row and  $h$  denotes the number of octagons in a column. Let  $P$  be a graph of  $TiO_2[g, h]$  with  $6h(g + 1)$  vertices and  $10gh + 8h$  edges. Figure 1 shows that the  $TiO_2$  vertex set is divided into four partitions, which are as follows:

$$\begin{aligned}V_2 &= \{v \in V(P) / \psi_P(v) = 2\}, |V_2| = 2gh + 4h \\ V_3 &= \{v \in V(P) / \psi_P(v) = 3\}, |V_3| = 2gh \\ V_4 &= \{v \in V(P) / \psi_P(v) = 4\}, |V_4| = 2h \\ V_5 &= \{v \in V(P) / \psi_P(v) = 5\}, |V_5| = 2gh\end{aligned}$$

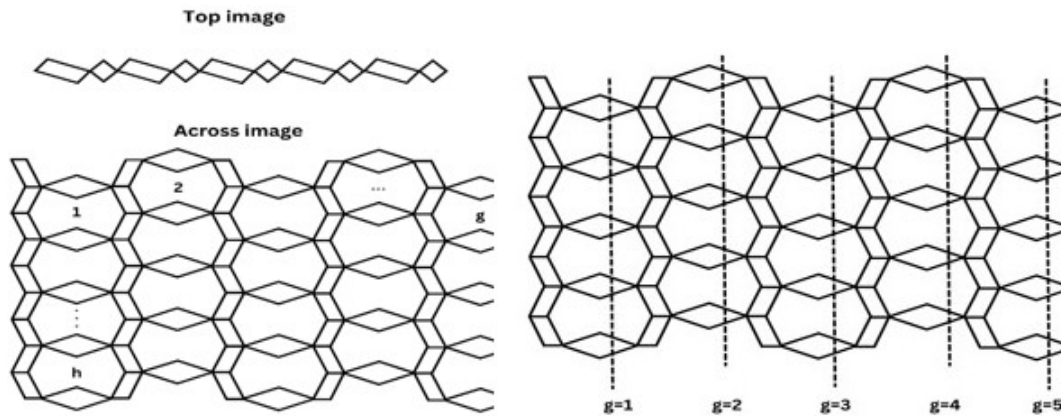
We obtain the three edge partitions of  $N$  using an algebraic method based on the sum of degrees of the end vertices as follows:

$$\begin{aligned} E_6 &= \{uv \in E(P) / \psi_P(u) = 2, \psi_P(v) = 4\}, |E_6| = 6h \\ E_7 &= \{uv \in E(P) / \psi_P(u) = 2, \psi_P(v) = 5\} \cup \\ &\quad \{uv \in E(P) / \psi_P(u) = 3, \psi_P(v) = 4\}, |E_7| = 4gh + 4h \\ E_8 &= \{uv \in E(P) / \psi_P(u) = 3, \psi_P(v) = 5\}, |E_8| = 6gh - 2h \end{aligned}$$

Similarly, We obtain the four edge partitions of  $N$  using an algebraic method based on the product of degrees of the end vertices as follows:

$$\begin{aligned} E_8 &= \{uv \in E(P) / \psi_P(u) = 2, \psi_P(v) = 4\}, |E_8| = 6h \\ E_{10} &= \{uv \in E(P) / \psi_P(u) = 2, \psi_P(v) = 5\}, |E_{10}| = 4gh + 2h \\ E_{12} &= \{uv \in E(P) / \psi_P(u) = 3, \psi_P(v) = 4\}, |E_{12}| = 2h \\ E_{15} &= \{uv \in E(P) / \psi_P(u) = 3, \psi_P(v) = 5\}, |E_{15}| = 6gh - 2h \end{aligned}$$

We determine Various topological indices of  $Tio_2$  nanotubes in the following theorems and corollaries.



**Figure 1: The graph of  $Tio_2[g, h]$ -nanotube**

**Theorem 3.1.** *The S-index of a titania nanotube is*

$$S(Tio_2) = 6800gh + 2176h$$

*Proof.* Utilizing the definition

$$\begin{aligned} S(Tio_2) &= \sum_{v \in V(P)} [\psi_P(v)^5] = 32|V_2| + 243|V_3| + 1024|V_4| + 3125|V_5| \\ &= 6800gh + 2176h \end{aligned}$$

□

**Theorem 3.2.** *The Modified Y-index of titania nanotube is*

$$MY(Tio_2) = 0.153gh + 0.257h$$

*Proof.* Utilizing the definition

$$MY(Tio_2) = \sum_{v \in V(P)} \frac{1}{[\psi_P(v)^4]} = \frac{1}{2^4}|V_2| + \frac{1}{3^4}|V_3| + \frac{1}{4^4}|V_4| + \frac{1}{5^4}|V_5| = 0.153gh + 0.257h$$

□

**Theorem 3.3.** *The Minus Y-index of titania nanotube is*

$$MY(TiO_2) = 1056gh + 448h$$

*Proof.* Utilizing the definition

$$\begin{aligned} MiY(TiO_2) &= \sum_{uv \in E(P)} [|\psi_P(u)^3 - \psi_P(v)^3|] = 56|E_8| + 117|E_{10}| + 37|E_{12}| + 98|E_{15}| \\ &= 1056gh + 448h \end{aligned}$$

□

**Theorem 3.4.** *The Sigma Y-index of titania nanotube is*

$$\sigma Y(TiO_2) = 112380gh + 29724h$$

*Proof.* Utilizing the definition

$$\sigma Y(TiO_2) = \sum_{uv \in E(P)} [\psi_P(u)^3 - \psi_P(v)^3]^2 = 112380gh + 29724h$$

□

**Theorem 3.5.** *The Modified Minus Y-index of titania nanotube is*

$$MMY(TiO_2) = 0.095gh + 0.158h$$

*Proof.* Utilizing the definition

$$MMY(TiO_2) = \sum_{uv \in E(P)} \frac{1}{|\psi_P(u)^3 - \psi_P(v)^3|} = 0.095gh + 0.158h$$

□

**Theorem 3.6.** *The Reduced Y-index of titania nanotube is*

$$ReY(TiO_2) = 546gh + 166h$$

*Proof.* Utilizing the definition

$$ReY(TiO_2) = \sum_{v \in V(P)} [\psi_P(v) - 1]^4 = 546gh + 166h$$

□

**Theorem 3.7.** *The Reduced Modified Y-index of titania nanotube is*

$$ReMY(TiO_2) = 2.133gh + 4.025h$$

*Proof.* Utilizing the definition

$$ReMY(TiO_2) = \sum_{v \in V(P)} \frac{1}{[\psi_P(v) - 1]^4} = 2.133gh + 4.025h$$

□

**Theorem 3.8.** *The Multiplicative Y-index of titania nanotube is*

$$\prod_Y(TiO_2) = 2^{8gh+32h} \times 3^{8gh} \times 5^{8gh} \times 19^{10gh}$$

*Proof.* Utilizing the definition

$$\prod_Y(TiO_2) = \prod_{v \in V(P)} [\psi_P(v)^4] = 2^{8gh+32h} \times 3^{8gh} \times 5^{8gh}$$

□

**Theorem 3.9.** *The Multiplicative Sigma Y-index of titania nanotube is*

$$\sigma_Y \prod (TiO_2) = 2^{12gh+32h} \times 7^{24gh+4h} \times 3^{16gh+8h} \times 13^{8gh+4h} \times 37^{4h}$$

*Proof.* Utilizing the definition

$$\begin{aligned} \sigma_Y \prod (TiO_2) &= \prod_{uv \in E(P)} [\psi_P(u)^3 - \psi_P(v)^3]^2 \\ &= 2^{12gh+32h} \times 7^{24gh+4h} \times 3^{16gh+8h} \times 13^{8gh+4h} \times 37^{4h} \end{aligned}$$

□

**Theorem 3.10.** *The Multiplicative Minus Y-index of titania nanotube is*

$$M_Y \prod (TiO_2) = 2^{6gh+16h} \times 7^{12gh+2h} \times 3^{8gh+4h} \times 13^{4gh+2h} \times 37^{2h}$$

*Proof.* Utilizing the definition

$$\begin{aligned} M_Y \prod (TiO_2) &= \prod_{uv \in E(P)} [|\psi_P(u)^3 - \psi_P(v)^3|] \\ &= 2^{18h} \times 7^{6gh+4h} \times 3^{8gh+4h} \times 13^{4gh+2h} \times 37^{2h} \end{aligned}$$

□

**Theorem 3.11.** *The Multiplicative Modified Minus Y-index of titania nanotube is*

$$MM_Y \prod (TiO_2) = \frac{1}{56}^{6h} \times \frac{1}{117}^{4gh+2h} \times \frac{1}{37}^{2h} \times \frac{1}{98}^{6gh-2h}$$

*Proof.* Utilizing the definition

$$\begin{aligned} MM_Y \prod (TiO_2) &= \prod_{uv \in E(P)} \frac{1}{|\psi_P(u)^3 - \psi_P(v)^3|} \\ &= \frac{1}{56}^{6h} \times \frac{1}{117}^{4gh+2h} \times \frac{1}{37}^{2h} \times \frac{1}{98}^{6gh-2h} \end{aligned}$$

□

**Theorem 3.12.** *The Multiplicative Reduced Y-index of titania nanotube is*

$$Re_Y \prod (TiO_2) = 2^{24gh} \times 3^{8h}$$

*Proof.* Utilizing the definition

$$Re_Y \prod (TiO_2) = \prod_{v \in V(P)} [\psi_P(v) - 1]^4 = 2^{24gh} \times 3^{8h}$$

□

**Theorem 3.13.** *The Multiplicative Reduced Modified Y-index of titania nanotube is*

$$ReM_Y \prod (TiO_2) = \frac{1}{2}^{24gh} \times \frac{1}{3}^{8h}$$

*Proof.* Utilizing the definition

$$ReM_Y \prod(Tio_2) = \prod_{v \in V(P)} \frac{1}{[\psi_P(v) - 1]^4} = \frac{1}{2}^{24gh} \times \frac{1}{3}^{8h}$$

□

**Proposition 3.1.** *The Modified S-index of titania nanotube is*

$$MS(Tio_2) = 0.071gh + 0.127h$$

**Proposition 3.2.** *The Minus S-index of titania nanotube is*

$$MS(Tio_2) = 5700gh + 1920h$$

**Proposition 3.3.** *The Sigma S-index of titania nanotube is*

$$\sigma S(Tio_2) = 3259140gh + 556740h$$

**Proposition 3.4.** *The Modified Minus S-index of titania nanotube is*

$$MMS(Tio_2) = 0.017gh + 0.036h$$

**Proposition 3.5.** *The Reduced S-index of titania nanotube is*

$$ReS(Tio_2) = 2114gh + 490h$$

**Proposition 3.6.** *The Reduced Modified S-index of titania nanotube is*

$$ReMS(Tio_2) = 2.064gh + 4.008h$$

**Proposition 3.7.** *The Multiplicative S-index of titania nanotube is*

$$\prod_S(Tio_2) = 2^{10gh+40h} \times 3^{10gh} \times 5^{10gh}$$

**Proposition 3.8.** *The Multiplicative Sigma S-index of titania nanotube is*

$$\sigma_S \prod(Tio_2) = 2^{60gh+28h} \times 3^{8gh+16h} \times 5^{20h} \times 7^{8gh+8h} \times 17^{12gh-4h} \times 29^{8gh+4h}$$

**Proposition 3.9.** *The Multiplicative Minus S-index of titania nanotube is*

$$M_S \prod(Tio_2) = 2^{30gh+14h} \times 3^{6h} \times 5^{10h} \times 7^{4gh+4h} \times 17^{6gh-2h} \times 87^{4gh+2h}$$

**Proposition 3.10.** *The Multiplicative Modified Minus S-index of titania nanotube is*

$$MM_S \prod(Tio_2) = \frac{1}{240}^{6h} \times \frac{1}{609}^{4gh+2h} \times \frac{1}{175}^{2h} \times \frac{1}{544}^{6gh-2h}$$

**Proposition 3.11.** *The Multiplicative Reduced S-index of titania nanotube is*

$$Re_S \prod(Tio_2) = 2^{30gh} \times 3^{10h}$$

**Proposition 3.12.** *The Multiplicative Reduced Modified S-index of titania nanotube is*

$$ReM_S \prod(Tio_2) = \frac{1}{2}^{30gh} \times \frac{1}{3}^{10h}$$



## 4. CONCLUSION

Topological indices are defined and used in many fields to investigate the properties of various objects such as atoms and molecules. Mathematicians and chemists have defined and studied a number of topological indices. Many new topological indices based on the  $Y$ -index and  $S$ -index are proposed in this study and these topological indices were determined for ( $TiO_2$ ) nanotubes. In future, we hope to investigate the topological indices of some new nanotubes in network and design sciences, which will be very useful in understanding their underlying chemical or physical properties.

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