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Research Paper

Some Graph Operations and Titania Nanotubes in Reformulated Y-index and Reformulated S-index

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Abstract

Topological indices are numerical values that correlate with a molecular graph's physical and chemical properties. Titania nanotubes are a well-known semiconductor with a wide range of technological applications including biomedical devices, dye-sensitized solar cells, and so on. We offer two new graph invariants in this study known as the 'reformulated Y-index' and 'reformulated S-index'. We calculate some special graphs and the reformulated Y-index and S-index for some graph operations like as join, Cartesian product, corona product, corona join product, subdivision vertex join and evaluate the titania nanotubes in reformulated indices.

1 Introduction

Topological and graph invariants based on distances between graph vertices are widely used for characterizing molecular graphs, establishing relationships between structural and 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 and graph indices. Graph theory has given chemists many useful tools, such as 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 of numerical coding of chemical structures with topological indices or topological coindices has been quite successful.

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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 two simple connected graphs, G_a and G_b, each with disjoint vertex and edge sets. For $i = a, b$, g_i and h_i represent the number of vertices and edges. The degree of a vertex v is the number of edges incident on the vertex v and is expressed as $d_G(v) = \chi_G(v)$ for every vertex $v \in V(G)$. In 1972, I. Gutman and N. Trinajstic [1] defined the first and second Zagreb index of a graph as :

$$M_1(G) = \sum_{v\in V(G)} [\chi_G(v)^2] = \sum_{uv\in E(G)} [\chi_G(u) + \chi_G(v)],$$
$$M_2(G) = \sum_{uv\in E(G)} [\chi_G(u)\chi_G(v)].$$

In 2015, B. Furtula and I. Gutman defined the F-index as [2]:

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

In 2020, Abdu Alameri and Noman AI-Naggar [3] introduced the Y-index, which is defined as:

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

In 2021, G. Priyadharsini et al. defined the S-index as [4]:

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

In 2004, A. Milicevic et al. [5] introduced the reformulated Zagreb index of a graph as:

$$EM_1(G) = \sum_{e\in E(G)} [\chi_G(e)^2] \text{ and } EM_2(G) = \sum_{e\sim f}[\chi_G(e)\chi_G(f)],$$

where $e \sim f$ means that the edges e and f share a common vertex in G, that is, they are adjacent. Note that the reformulated Zagreb indices of a graph G coincide with the ordinary Zagreb indices of the line graph of G [6–11].
In 2017, H. Aram and N. Dehgardi [12] defined the reformulated F-index of a graph as:

$$RF(G) = \sum_{e\in E(G)} [\chi_G(e)^3].$$

We now first introduce the reformulated Y-index of a graph, which is derived from the Y-indices by replacing vertex degrees with edge degrees, where the degree of an edge $e = uv$ is defined as the sum of the degrees of the edge's end vertices minus 2 and is denoted by $\chi_G(e) = \chi_G(u) + \chi_G(v) - 2$. Thus the reformulated Y-index of a graph is defined as:

$$RY(G) = \sum_{e\in E(G)} [\chi_G(e)^4].$$

Next we introduce the reformulated S-index of a graph, which is derived from the S-indices by replacing vertex degrees with edge degrees and is defined as:

$$RS(G) = \sum_{e\in E(G)} [\chi_G(e)^5].$$

Note that the reformulated F, Y, and S indices of a graph G coincide with the ordinary F, Y, and S indices of the line graph of G. In 2017, H. Aram and N. Dehgardi [12] explained the graph operations in F-index. D. Nilanjan [13] determined the graph operations in Zagreb indices in 2015. M. Rezaei and W. Gao [14] explained the hyper Zagreb index and M-polynomial of (Tio_2) in 2017. A. Subhashini and J. Baskar [15] determined the topological indices based on vertex degree of (Tio_2) in 2018. N. De [16] find the titania nanotube for some topological properties in 2016. In this paper, we evaluated some special graphs and some expressions for the reformulated Y-index and reformulated S-index of various graph operations and titania nanotubes (Tio_2).

2 Main results

The join of graph [2, 3]:

$$\begin{aligned} |V(G_a+G_b)| &= |V(G_a)|+|V(G_b)| = g_a+g_b, \\ |E(G_a+G_b)| &= |E(G_a)|+|E(G_b)|+|V(G_a)||V(G_b)| = h_a+h_b+g_ag_b. \end{aligned}$$

The degree of a vertex v of G_a+G_b is defined as:

$$\chi_{G_a+G_b}(v) = \begin{cases} \chi_{G_a}(v)+g_b, & v\in V(G_a), \\ \chi_{G_b}(v)+g_a, & v\in V(G_b). \end{cases}$$

Theorem 2.1. *The reformulated Y-index of G_a+G_b is determined by*

$$\begin{aligned} RY(G_a+G_b) &= RY(G_a)+RY(G_b)+8[g_bRF(G_a)+g_aRF(G_b)] \\ &+ 24[g_b^2EM_1(G_a)+g_a^2EM_1(G_b)]-64[g_b^3h_a+g_a^3h_b]+16[g_b^4h_a+g_a^4h_b] \\ &+ g_bY(G_a)+g_aY(G_b)+F(G_a)[8h_b+4g_b(g_a+g_b-2)] \\ &+ F(G_b)[8h_a+4g_a(g_a+g_b-2)]+M_1(G_a)(g_a+g_b-2)[24h_b+6g_b(g_a+g_b-2)] \\ &+ M_1(G_b)(g_a+g_b-2)[24h_a+6g_a(g_a+g_b-2)]+48h_ah_b(g_a+g_b-2)^2 \\ &+ 6M_1(G_a)M_1(G_b)+8(g_a+g_b-2)^3[h_ag_b+g_ah_b]+g_ag_b(g_a+g_b-2)^4 \\ &+ 32M_1(G_a)g_b^3+32M_1(G_b)g_a^3. \end{aligned}$$

Proof.

$$\begin{aligned} RY(G_a+G_b) &= \sum_{uv\in E(G_a+G_b)} (\chi_{G_a+G_b}(u)+\chi_{G_a+G_b}(v)-2)^4 \\ &= \sum_{uv\in E(G_a)} (\chi_{G_a+G_b}(u)+\chi_{G_a+G_b}(v)-2)^4 \\ &+ \sum_{uv\in E(G_b)} (\chi_{G_a+G_b}(u)+\chi_{G_a+G_b}(v)-2)^4 \\ &+ \sum_{u\in V(G_a)}\sum_{v\in V(G_b)} (\chi_{G_a+G_b}(u)+\chi_{G_a+G_b}(v)-2)^4 \\ &= K_1+K_2+K_3. \end{aligned}$$

We begin by calculating K_1, we've

$$\begin{aligned} K_1 &= \sum_{uv\in E(G_a)} (\chi_{G_a}(u)+\chi_{G_a}(v)-2+2g_b)^4 \\ &= RY(G_a)+8g_bRF(G_a)+24g_b^2EM_1(G_a)+32M_1(G_a)g_b^3-64g_b^3h_a+16g_b^4h_a. \end{aligned}$$

After that, we compute K_2, we've

$$\begin{aligned} K_2 &= \sum_{uv\in E(G_b)} (\chi_{G_b}(u)+\chi_{G_b}(v)-2+2g_a)^4 \\ &= RY(G_b)+8g_aRF(G_b)+24g_a^2EM_1(G_b)+32M_1(G_b)g_a^3-64g_a^3h_b+16g_a^4h_b. \end{aligned}$$

Finally, we compute K_3, we've

$$\begin{aligned} K_3 &= \sum_{u\in V(G_a)}\sum_{v\in V(G_b)} (\chi_{G_a}(u)+\chi_{G_b}(v)-2+g_a+g_b)^4 \\ &= g_bY(G_a)+g_aY(G_b)+F(G_a)[8h_b+4g_b(g_a+g_b-2)]+F(G_b)[8h_a+4g_a(g_a+g_b-2)] \\ &+ M_1(G_a)(g_a+g_b-2)[24h_b+6g_b(g_a+g_b-2)] \\ &+ M_1(G_b)(g_a+g_b-2)[24h_a+6g_a(g_a+g_b-2)]+48h_ah_b(g_a+g_b-2)^2+6M_1(G_a)M_1(G_b) \\ &+ 8(g_a+g_b-2)^3[h_ag_b+g_ah_b]+g_ag_b(g_a+g_b-2)^4. \end{aligned}$$

Attaching K_1, K_2, K_3, we obtain the evaluated outcome. ■

Theorem 2.2. *The reformulated S-index of G_a+G_b is determined by*

$$\begin{aligned} RS(G_a+G_b) &= RS(G_a)+RS(G_b)+10[g_bRY(G_a)+g_aRY(G_b)]+40[g_b^2RF(G_a) \\ &+g_a^2RF(G_b)]+80[g_b^3EM_1(G_a)+g_a^3EM_1(G_b)]-160[g_b^4h_a+g_a^4h_b] \\ &+32[g_b^5h_a+g_a^5h_b]+M_1(G_a)[80g_b^4+10F(G_b)+30M_1(G_b)(g_a+g_b-2) \\ &+60h_b(g_a+g_b-2)^2+10g_b(g_a+g_b-2)^3]+M_1(G_b)[80g_a^4+10F(G_a) \\ &+60h_a(g_a+g_b-2)^2+10g_a(g_a+g_b-2)^3]+g_bS(G_a)+g_aS(G_b)+Y(G_a) \\ &[10h_b+5g_b(g_a+g_b-2)]+Y(G_b)[10h_a+5g_a(g_a+g_b-2)]+F(G_a) \\ &[40h_b(g_a+g_b-2)+10g_b(g_a+g_b-2)^2]+F(G_b)[40h_a(g_a+g_b-2) \\ &+10g_a(g_a+g_b-2)^2]+80h_ah_b(g_a+g_b-2)^3+10(g_a+g_b-2)^4 \\ &(h_ag_b+h_bg_a)+g_ag_b(g_a+g_b-2)^5. \end{aligned}$$

The Cartesian product of graph [2, 5]:

$$\begin{aligned} |V(G_a\times G_b)| &= |V(G_a)||V(G_b)| = g_ag_b, \\ |E(G_a\times G_b)| &= |E(G_a)||V(G_b)|+|E(G_b)||V(G_a)| = h_ag_b+h_bg_a. \end{aligned}$$

The degree of a vertex $v=(x,y)$ of $G_a\times G_b$ is defined as:

$$\chi_{G_a\times G_b}(x,y)=\chi_{G_a}(x)+\chi_{G_b}(y).$$

Theorem 2.3. *The reformulated Y-index of $G_a\times G_b$ is determined by*

$$\begin{aligned} RY(G_a\times G_b) &= g_bRY(G_a)+g_aRY(G_b)+16[h_bRF(G_a)+h_aRF(G_b)] \\ &+ 24[M_1(G_b)EM_1(G_a)+M_1(G_a)EM_1(G_b)]+32[(M_1(G_b)-2h_b)F(G_a) \\ &- (M_1(G_a)-2h_a)F(G_b)]+16[h_bY(G_a)+h_aY(G_b)]. \end{aligned}$$

Proof.

$$\begin{aligned} RY(G_a\times G_b) &= \sum_{(u,x)(v,y)\in E(G_a\times G_b)} (\chi_{G_a\times G_b}(u,x)+\chi_{G_a\times G_b}(v,y)-2)^4 \\ &= \sum_{u\in V(G_a)}\sum_{xy\in E(G_b)} (\chi_{G_a\times G_b}(u,x)+\chi_{G_a\times G_b}(v,y)-2)^4 \\ &+ \sum_{x\in V(G_b)}\sum_{uv\in E(G_a)} (\chi_{G_a\times G_b}(u,x)+\chi_{G_a\times G_b}(v,y)-2)^4 \\ &= K_1+K_2. \end{aligned}$$

We begin by calculating K_1, we've

$$\begin{aligned} K_1 &= \sum_{u\in V(G_a)}\sum_{xy\in E(G_b)} (\chi_{G_b}(x)+\chi_{G_b}(y)-2+2\chi_{G_a}(u))^4 \\ &= g_aRY(G_b)+16h_aRF(G_b)+24M_1(G_a)EM_1(G_b) \\ &+ 32(M_1(G_b)-2h_b)F(G_a)+16h_bY(G_a). \end{aligned}$$

After that, we compute K_2, we've

$$\begin{aligned} K_2 &= \sum_{x\in V(G_b)}\sum_{uv\in E(G_a)} (\chi_{G_a}(u)+\chi_{G_a}(v)-2+2\chi_{G_b}(x))^4 \\ &= g_bRY(G_a)+16h_bRF(G_a)+24M_1(G_b)EM_1(G_a) \\ &+ 32(M_1(G_a)-2h_a)F(G_b)+16h_aY(G_b). \end{aligned}$$

Attaching K_1, K_2, we obtain the evaluated outcome. ■

Theorem 2.4. *The reformulated S-index of $G_a \times G_b$ is determined by*

$$\begin{aligned} RS(G_a\times G_b) &= g_bRS(G_a)+g_aRS(G_b)+20[h_bRY(G_a)+h_aRY(G_b)] \\ &+ M_1(G_a)[40RF(G_b)+80Y(G_b)]+80[EM_1(G_b)F(G_a)+EM_1(G_a)F(G_b)] \\ &+ M_1(G_b)[40RF(G_a)+80Y(G_a)]-160[h_bY(G_a)+h_aY(G_b)] \\ &+ 32[h_bS(G_a)+h_aS(G_b)]. \end{aligned}$$

The corona product of graph [3, 12]:

$$\begin{aligned} |V(G_a\odot G_b)| &= |V(G_a)|+|V(G_a)||V(G_b)| = g_a+g_ag_b, \\ |E(G_a\odot G_b)| &= |E(G_a)|+|V(G_a)||E(G_b)|+|V(G_a)||V(G_b)| = h_a+g_ah_b+g_ag_b. \end{aligned}$$

The degree of a vertex v of $G_a \odot G_b$ is defined as:

$$\chi_{G_a\odot G_b}(v) = \begin{cases} \chi_{G_a}(v)+g_b, & v\in V(G_a), \\ \chi_{G_b}(v)+1, & v\in V(G_{b,i}). \end{cases}$$

Theorem 2.5. *The reformulated Y-index of $G_a \odot G_b$ is determined by*

$$\begin{aligned} RY(G_a\odot G_b) &= RY(G_a)+g_aRY(G_b)+8[g_bRF(G_a)+g_aRF(G_b)] \\ &+ 24[g_b^2EM_1(G_a)+g_aEM_1(G_b)]+16[g_b^4h_a+g_ah_b]-64[g_b^3h_a+g_ah_b] \\ &+ 32[M_1(G_a)g_b^3+M_1(G_b)g_a]+6M_1(G_a)M_1(G_b) \\ &+ M_1(G_a)[6g_b(g_b-1)^2+24(g_b-1)h_b] \\ &+ M_1(G_b)[6g_a(g_b-1)^2+24(g_b-1)h_a]+g_aY(G_b)+g_bY(G_a) \\ &+ F(G_a)[8h_b+4(g_b-1)g_b]+F(G_b)[8h_a+4(g_b-1)g_a]+48h_ah_b(g_b-1)^2 \\ &+ 8(g_b-1)^3[h_ag_b+g_ah_b]+(g_b-1)^4g_ag_b. \end{aligned}$$

Proof.

$$\begin{aligned}
RY(G_a \odot G_b) &= \sum_{uv \in E(G_a \odot G_b)} (\chi_{G_a \odot G_b}(u) + \chi_{G_a \odot G_b}(v) - 2)^4 \\
&= \sum_{e \in E_1} (\chi_{G_a \odot G_b}(u_k) + \chi_{G_a \odot G_b}(v_k) - 2)^4 \\
&+ \sum_{e \in E_2} (\chi_{G_a \odot G_b}(u_l) + \chi_{G_a \odot G_b}(v_l) - 2)^4 \\
&+ \sum_{e \in E_3} (\chi_{G_a \odot G_b}(u_k) + \chi_{G_a \odot G_b}(v_l) - 2)^4 \\
&= S_1 + S_2 + S_3.
\end{aligned}$$

We begin by calculating S_1, we've

$$\begin{aligned}
S_1 &= \sum_{u_k v_k \in E(G_a)} (\chi_{G_a}(u_k) + \chi_{G_a}(v_k) - 2 + 2(g_b - 1))^4 \\
&= RY(G_a) + 8g_b RF(G_a) + 24g_b^2 EM_1(G_a) + 32M_1(G_a)g_b^3 - 64g_b^3 h_a + 16g_b^4 h_a.
\end{aligned}$$

After that, we compute S_2, we've

$$\begin{aligned}
S_2 &= \sum_{k=1}^{g_a} \sum_{u_l v_l \in E(G_b)} (\chi_{G_b}(u_l) + \chi_{G_b}(v_l) - 2 + 2)^4 \\
&= g_a RY(G_b) + 8g_a RF(G_b) + 24g_a EM_1(G_b) + 32M_1(G_b)g_a - 64g_a h_b + 16g_a h_b.
\end{aligned}$$

Finally, we compute S_3, we've

$$\begin{aligned}
S_3 &= \sum_{k=1}^{g_a} \sum_{l=1}^{g_b} (\chi_{G_a}(u_k) + \chi_{G_b}(v_l) + g_b - 1)^4 \\
&= 6M_1(G_a)M_1(G_b) + M_1(G_a)[6g_b(g_b - 1)^2 + 24(g_b - 1)h_b] \\
&+ M_1(G_b)[6g_a(g_b - 1)^2 + 24(g_b - 1)h_a] + g_a Y(G_b) + g_b Y(G_a) + F(G_a)[8h_b + 4(g_b - 1)g_b] \\
&+ F(G_b)[8h_a + 4(g_b - 1)g_a] + 48h_a h_b (g_b - 1)^2 + 8(g_b - 1)^3[h_a g_b + g_a h_b] + (g_b - 1)^4 g_a g_b.
\end{aligned}$$

Attaching S_1, S_2, S_3, we obtain the evaluated outcome. ■

Theorem 2.6. *The reformulated S-index of $G_a \odot G_b$ is determined by*

$$\begin{aligned}
RS(G_a \odot G_b) &= RS(G_a) + g_a RS(G_b) + 10[g_b RY(G_a) + g_a RY(G_b)] \\
&+ 40[g_b^2 RF(G_a) + g_a RF(G_b)] + 80[g_b^3 EM_1(G_a) + g_a EM_1(G_b)] \\
&- 160[g_b^4 h_a + g_a h_b] + 32[g_b^5 h_a + g_a h_b] \\
&+ M_1(G_a)[80g_b^4 + 10F(G_b) + 30(g_b - 1)M_1(G_b) + 60(g_b - 1)^2 h_b + 10(g_b - 1)^3 g_b] \\
&+ M_1(G_b)[80g_a + 10F(G_a) + 60(g_b - 1)^2 h_a + 10(g_b - 1)^3 g_a] + g_a S(G_b) + g_b S(G_a) \\
&+ Y(G_a)[10h_b + 5(g_b - 1)g_b] + Y(G_b)[10h_a + 5(g_b - 1)g_a] \\
&+ F(G_a)[40(g_b - 1)h_b + 10(g_b - 1)^2 g_b] + F(G_b)[40(g_b - 1)h_a + 10(g_b - 1)^2 g_a] \\
&+ 80(g_b - 1)^3 h_a h_b + (g_b - 1)^4[10h_a g_b + 10h_b g_a] + (g_b - 1)^5 g_a g_b.
\end{aligned}$$

The corona join product of graph [4]:
The degree of a vertex v of $G_a \bigoplus G_b$ is defined as:

$$\chi_{G_a \bigoplus G_b}(v) = \begin{cases} \chi_{G_a}(v) + g_a g_b, & v \in V(G_a), \\ \chi_{G_b}(v) + g_a, & v \in V(G_b). \end{cases}$$

Lemma 2.7. *The Y-index of $G_a \bigoplus G_b$ is determined by*

$$\begin{aligned} Y(G_a \bigoplus G_b) &= Y(G_a) + g_a Y(G_b) + 4[F(G_a) g_a g_b + F(G_b) g_a^2] \\ &+ 6[M_1(G_a) g_a^2 g_b^2 + M_1(G_b) g_a^3] + 8[h_a g_a^3 g_b^3 + h_b g_a^4] + g_a^5 [g_b^4 + g_b]. \end{aligned}$$

Theorem 2.8. *The reformulated Y-index of $G_a \bigoplus G_b$ is determined by*

$$\begin{aligned} RY(G_a \bigoplus G_b) &= RY(G_a) + g_a RY(G_b) + 8[g_a g_b RF(G_a) + g_a^2 RF(G_b)] + 16[g_a^4 g_b^4 h_a + g_a^5 h_b] \\ &+ 24[g_a^2 g_b^2 EM_1(G_a) + g_a^3 EM_1(G_b)] + M_1(G_a)[32 g_a^3 g_b^3 + 24 g_a h_b (g_a + g_a g_b - 2) \\ &+ 6 g_a g_b (g_a + g_a g_b - 2)^2] - 64[g_a^3 g_b^3 h_a + h_b g_a^4] \\ &+ M_1(G_b)[32 g_a^4 + 6 M_1(G_a) g_a + 24 g_a h_a (g_a + g_a g_b - 2) + 6 g_a^2 g_b (g_a + g_a g_b - 2)^2] \\ &+ g_a g_b Y(G_a) + g_a^2 Y(G_b) + F(G_a)[8 g_a h_b + 4 g_a g_b (g_a + g_a g_b - 2)] \\ &+ F(G_b)[8 g_a h_a + 4 g_a^2 (g_a + g_a g_b - 2)] + g_b g_a^2 (g_a + g_a g_b - 2)^4 \\ &+ 48 h_a h_b g_a (g_a + g_a g_b - 2)^2 + 8 (g_a + g_a g_b - 2)^3 (h_a + h_b). \end{aligned}$$

Proof.

$$\begin{aligned} RY(G_a \bigoplus G_b) &= \sum_{uv \in E(G_a \bigoplus G_b)} (\chi_{G_a \bigoplus G_b}(u) + \chi_{G_a \bigoplus G_b}(v) - 2)^4 \\ &= \sum_{uv \in E(G_a)} (\chi_{G_a \bigoplus G_b}(u) + \chi_{G_a \bigoplus G_b}(v) - 2)^4 \\ &+ g_a \sum_{uv \in E(G_b)} (\chi_{G_a \bigoplus G_b}(u) + \chi_{G_a \bigoplus G_b}(v) - 2)^4 \\ &+ g_a \sum_{u \in V(G_a)} \sum_{v \in V(G_b)} (\chi_{G_a \bigoplus G_b}(u) + \chi_{G_a \bigoplus G_b}(v) - 2)^4 \\ &= \sum_{uv \in E(G_a)} (\chi_{G_a}(u) + \chi_{G_a}(v) - 2 + 2 g_a g_b)^4 \\ &+ g_a \sum_{uv \in E(G_b)} (\chi_{G_b}(u) + \chi_{G_b}(v) - 2 + 2 g_a)^4 \\ &+ g_a \sum_{u \in V(G_a)} \sum_{v \in V(G_b)} (\chi_{G_a}(u) + \chi_{G_b}(v) + (g_a + g_a g_b - 2))^4. \end{aligned}$$

We obtain the evaluated outcome. ■

Theorem 2.9. *The reformulated S-index of $G_a \bigoplus G_b$ is determined by*

$$\begin{aligned} RS(G_a \bigoplus G_b) &= RS(G_a) + g_a RS(G_b) + 10[g_a g_b RY(G_a) + g_a^2 RY(G_b)] \\ &+ 40[g_a^2 g_b^2 RF(G_a) + g_a^3 RF(G_b)] + 80[g_a^3 g_b^3 EM_1(G_a) + g_a^4 EM_1(G_b)] \\ &+ 32(g_a^5 g_b^5 + g_a^6) - 160[h_a g_a^4 g_b^4 + h_b g_a^5] + M_1(G_a)[80 g_a^4 g_b^4 + 10 g_a F(G_b) + \\ &\quad 30(g_a + g_a g_b - 2) M_1(G_b) g_a + 60 g_a h_b (g_a + g_a g_b - 2)^2 + 10 g_a g_b (g_a + g_a g_b - 2)^3] \\ &+ M_1(G_b)[80 g_a^5 + 10 g_a F(G_a) + 60 g_a h_a (g_a + g_a g_b - 2)^2 + 10(g_a + g_a g_b - 2)^3 g_a^2] \\ &+ g_a g_b S(G_a) + g_a^2 S(G_b) + Y(G_a)[10 h_b g_a + 5(g_a + g_a g_b - 2) g_a g_b] \\ &+ Y(G_b)[10 h_a g_a + 5(g_a + g_a g_b - 2) g_a^2] + F(G_a)[40(g_a + g_a g_b - 2) g_a h_b + 10 g_a g_b \\ &\quad (g_a + g_a g_b - 2)^2] + F(G_b)[40(g_a + g_a g_b - 2) g_a h_a + 10 g_a^2 (g_a + g_a g_b - 2)^2] \\ &+ 80 g_a h_a h_b (g_a + g_a g_b - 2)^3 + 10 g_a (g_a + g_a g_b - 2)^4 (h_a g_b + g_a h_b) \\ &+ (g_a + g_a g_b - 2)^5 g_a^2 g_b. \end{aligned}$$

The subdivision vertex join of graph [4]:
The degree of a vertex v of $G_a \boxplus G_b$ is defined as:

$$\chi_{G_a \boxplus G_b}(v) = \begin{cases} \chi_{G_a}(v), & v \in V(G_a), \\ 2 + g_b, & v \in V_s(G_a), \\ \chi_{G_b}(v) + h_a, & v \in V(G_b). \end{cases}$$

Lemma 2.10. *The Y-index of $G_a \boxplus G_b$ is determined by*

$$Y(G_a \boxplus G_b) = Y(G_a) + h_a(2 + g_b)^4 + Y(G_b) + 4F(G_b)h_a + 6M_1(G_b)h_a^2 + 8h_b h_a^3 + g_b h_a^4.$$

Theorem 2.11. *The reformulated Y-index of $G_a \boxplus G_b$ is determined by*

$$\begin{aligned} RY(G_a \boxplus G_b) &= \sum_{\substack{uv \in E(S(G_a)) \\ u \in V(G_a) \\ v \in V_s(G_a)}} \left[\chi_{G_a}(u)^4 + 4 g_b \chi_{G_a}(u)^3 + 6 \chi_{G_a}(u)^2 g_b^2 + 4 \chi_{G_a}(u) g_b^3\right] \\ &+ g_b^4 h_a^{'} + RY(G_b) + 16 h_a^4 h_b + 8 RF(G_b) h_a + 24 h_a^2 EM_1(G_b) \\ &+ M_1(G_b)[38 h_a^3 + 6 g_b^2 h_a + 12 h_a^2 g_b] - 64 h_a^3 h_b + g_b^5 h_a + h_a Y(G_b) + h_a^5 g_b \\ &+ F(G_b[4 h_a^2 + 4 g_b h_a] + 8 h_a^4 h_b + 8 g_b^3 h_a h_b + 4 h_a^2 g_b^4 \\ &+ g_b h_a^2 [6 g_b^2 h_a + 24 g_b h_b + 4 g_b h_a^2 + 24 h_a h_b]. \end{aligned}$$

Proof.

$$\begin{aligned} RY(G_a \boxplus G_b) &= \sum_{uv \in E(G_a \boxplus G_b)} (\chi_{G_a \boxplus G_b}(u) + \chi_{G_a \boxplus G_b}(v) - 2)^4 \\ &= \sum_{\substack{uv \in E(S(G_a)) \\ u \in V(G_a) \\ v \in V_s(G_a)}} (\chi_{G_a}(u) + 2 + g_b - 2)^4 \\ &+ \sum_{uv \in E(G_b)} (\chi_{G_b}(u) + 2h_a + \chi_{G_b}(v) - 2)^4 \\ &+ \sum_{\substack{uv \in E(G_a \boxplus G_b)) \\ u \in V_s(G_a) \\ v \in V(G_b)}} (2 + g_b + \chi_{G_b}(v) + h_a)^4. \end{aligned}$$

We obtain the evaluated outcome. ■

Theorem 2.12. *The reformulated S-index of $G_a \boxplus G_b$ is determined by*

$$\begin{aligned} & RS(G_a \boxplus G_b) \\ = & \sum_{\substack{uv \in E(S(G_a)) \\ u \in V(G_a) \\ v \in V_s(G_a)}} \left[\chi_{G_a}(u)^5 + 5\chi_{G_a}(u)^4 g_b + 10 g_b^2 \chi_{G_a}(u)^3 + 10\chi_{G_a}(u)^2 g_b^3 + 5\chi_{G_a}(u) g_b^4\right] \\ + & g_b^5 h_a^{'} + RS(G_b) + 10RY(G_b)h_a + 40RF(G_b)h_a^2 - 160h_a^4 h_b \\ + & 80h_a^3 EM_1(G_b) + 32h_a^5 + M_1(G_b)[90h_a^4 + 6h_a^3 + 30h_a^2 g_b^2 + 10g_b^3 h_a] \\ + & h_a S(G_b) + 5Y(G_b)(h_a^2 + h_a g_b) + F(G_b)[10h_a^3 + 10g_b^2 h_a + 20h_a^2 g_b] + h_b[10h_a^5 + 40h_a^4 g_b] \\ + & g_b(h_a^5 + h_a^6) + 10[h_a^4 g_b^3 + h_a^3 g_b^4] + 60g_b^2 h_a^3 h_b + 40g_b^3 h_a^2 h_b + 5g_b^4[2h_a h_b + h_a^2 g_b] + g_b^6 h_a. \end{aligned}$$

In the Corollary 2.13 and 2.14, we estimated the reformulated Y-index and reformulated S-index of some special graphs with n vertices, such as Path, Cycle, Star, Wheel, and Ladder graphs.

Corollary 2.13. *For a graph G with n vertices, we have*

a) $RY(P_n) = 16n - 46,\ n \geq 3,$

b) $RY(C_n) = 16n,\ n \geq 3,$

c) $RY(S_n) = (n-2)^4(n-1),\ n > 4,$

d) $RY(W_n) = 256(n-1) + n^4(n-1),\ n > 3,$

e) $RY(L_n) = 768n - 1692,\ n > 3.$

Corollary 2.14. *For a graph G with n vertices, we have*

a) $RS(P_n) = 32n - 94,\ n \geq 3,$

b) $RS(C_n) = 32n,\ n \geq 3,$

c) $RS(S_n) = (n-2)^5(n-1),\ n > 4,$

d) $RS(W_n) = 1024(n-1) + n^5(n-1),\ n > 3,$

e) $RS(L_n) = 3072n - 7156,\ n > 3.$

3 Titania (Tio_2) nanotubes

Figure 1 depicts the titania nanotube graph, where g denotes the number of octagons in a row and h denotes the number of octagons in a column. Let G 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:

$$\begin{aligned} V_2 &= \{v \in V(G) \mid \chi_G(v) = 2\},\ |V_2| = 2gh + 4h, \\ V_3 &= \{v \in V(G) \mid \chi_G(v) = 3\},\ |V_3| = 2gh, \\ V_4 &= \{v \in V(G) \mid \chi_G(v) = 4\},\ |V_4| = 2h, \\ V_5 &= \{v \in V(G) \mid \chi_G(v) = 5\},\ |V_5| = 2gh. \end{aligned}$$

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

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

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

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

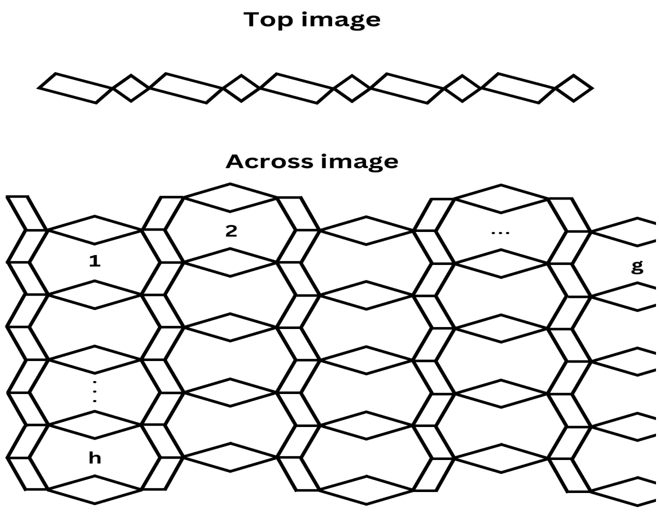

Figure 1: The graph of titania nanotube.

We determine reformulated Y-index and reformulated S-index of Tio_2 nanotubes in the following propositions.

Proposition 3.1. *The reformulated Y-index of titania nanotube is*

$$RY(Tio_2) = 10276gh + 1444h.$$

Proof. Utilizing the definition

$$RY(Tio_2) = \sum_{e \in E(G)} [\chi_G(e)^4] = 4^4\,|E_8| + 5^4\,|E_{10}| + 5^4\,|E_{12}| + 6^4\,|E_{15}| = 10276gh + 1444h,$$

we obtain the evaluated outcome. ■

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

$$RS(Tio_2) \quad = \quad 59156gh + 3092h.$$

Proof. Utilizing the definition

$$RS(Tio_2) \quad = \quad \sum_{e \in E(G)} [\chi_G(e)^5] = 4^5\,|E_8| + 5^5\,|E_{10}| + 5^5\,|E_{12}| + 6^5\,|E_{15}| = 59156gh + 3092h,$$

we obtain the evaluated outcome. ■

4 Concluding remarks

Topological indices are defined and used in many fields to investigate the properties of various objects such as atoms and molecules. We investigated some special graphs and the reformulated Y-index and reformulated S-index of various graph operations such as join, Cartesian product, corona product, subdivision vertex join, and corona join product and determined the reformulated indices of titania nanotubes (Tio_2) in this work.

Author Contributions. Kayalvizhi Gokulathilagan developed the theoretical formalism and performed the analytic calculations. Nagarajan Sethumadhavan supervised the project. All authors discussed the results and contributed to the final manuscript.

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