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Calculation of Revan topological indices in $TiO_2[m, n]$ nanotubes

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Abstract

Titania nanotubes are one of the most essential and practical compounds in materials science that have many applications in the production of catalytic materials, gas sensors, biomedical devices, solar cells etc.

In this article, the graph of Titania nanotubes is investigated. By providing a method to obtain the degree of vertices in the section of the corresponding nanotube, the topological indices of Revan and its Hyper Revan are calculated. Next, the Revan and Hyper Revan indices in line graph of Titania nanotubes are also computing. To compare the obtained values, diagrams of Revan and Hyper Revan indices are drawn.

Subject Classification: *(2010) 05C90, 92E10, 05C07, 92E20, 82D80.*

Keywords: *Revan indices, Hyper Revan indices, Titania nanotubes, Line graph.*

1. Introduction

Graph theory is used in chemistry for modeling. Study in nanoscale leads to drastic changes in material properties. Numerical calculations are of particular importance in nanoscale simulations.

In nanoscience, the study of atomic, molecular, and macromolecular dimensions was discussed, and research in these dimensions leads to a drastic change in the properties of materials.

At the nanoscale, materials exhibit quantum properties that are often not measurable in practice. For this purpose, the desired systems should be mathematically modeled and the relevant equations should be solved for them. Since accurate solutions of equations are not possible in most

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cases, numerical solutions should be used instead of analytical or exact solutions to solve equations.

In a molecular graph, the topological index is expressed as an actual number, and this number is attributed to the graphs, uniform with that molecule.

The topological index also indicates some of the properties of the molecule.

In 1947, the first and most studied topological index was introduced by Weiner [10]. One of the practical tools in studying the structure and properties of a molecule is the topological indices of its chemical graph.

In this article, the Revan and Hyper Revan indices in the graph of Titania nanotubes are investigated.

2. Preliminaries

This section provides some of the required definitions. Suppose $H = (V, E)$ is a simple and connected graph. We represent the set of edges with $E(H)$ and the number of edges with $|E(H)|$ and the set of vertices with $V(H)$ and the number of vertices with $|V(H)|$.

We denote the degree of vertex x by d_x and if there is an edge between two vertices x and y, we denoted it by $xy \in E(H)$.

The first and second Indices of Zagreb were first introduced by Guttman et. al. These Indices have been used as branching Indices. Zagreb indices have found many applications in QSPR and QSAR studies [5].

Motivated by the definitions of Zagreb indices and their wide applications, Revan indices for graph H were defined by V.R. Kulli in 2017 [7][4].

In graph H, we denote the minimum vertex degree by $\delta(H)$ and the maximum vertex degree by $\Delta(H)$. Then the degree of Revan for vertex x in graph H is expressed as follows:

$$r_H(x) = \Delta(H) + \delta(H) - d_x.$$

Definition 2.1: In graph H, the first and second Revan index can be defined as follows:

$$R_1(H) = \sum_{i=1}^{|E(H)|} \psi_i,$$
$$R_2(H) = \sum_{i=1}^{|E(H)|} \psi'_i.$$

Which are in $\psi_i = [r_G(u) + r_G(v)]$ and $\psi'_i = r_G(u) r_G(v)$.

Definition 2.2: In graph H, the first and second Hyper Revan index can be defined as follows:

$$HR_1(H) = \sum_{i=1}^{|E(H)|} \psi_i'',$$
$$HR_2(H) = \sum_{i=1}^{|E(H)|} \psi_i'''.$$

Which are in $\psi_i'' = [r_H(x) + r_H(y)]^2$ and $\psi_i''' = (r_H(x) r_H(y))^2$.

Definition 2.3: In a non-empty graph H, if each edge is considered as a vertex and the two vertices are connected, if the corresponding edges of the two vertices are adjacent to H, the resulting graph is denoted by $L(H)$ and is called the line graph of H [2].

3. The structure of Titania nanotube $TiO_2[m, n]$

In this section, the structure of the Titania nanotube $TiO_2[m, n]$ graph is studied to calculate the Revan indices. Carbon nanotubes are extremely strong and flexible at the same time. In materials science, Titania is a well-known semiconductor and has several technologies [11].

Over the last 15 years, Titania nanotubes have been systematically synthesized using various methods and have several technological applications such as biomedical devices, color-sensitive solar cells etc [2].

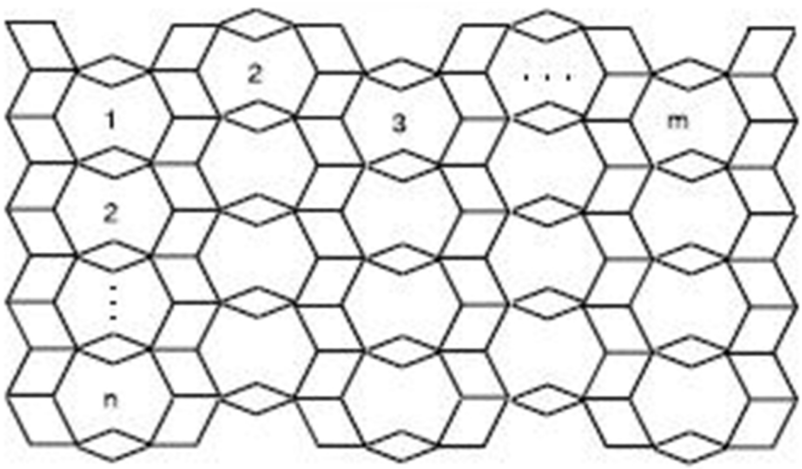

Figure 1

The molecular graph of Titania nanotube where *m* represents the number of octagons in a row and n represents the number of octagons in a column of Titania nanotubes

Since the growth mechanism for Titania nanotubes is not yet well understood, comprehensive theoretical studies on them are attracting more attention.

One of the characteristics of Titania nanotube sheets is the considerable stability of its atomic multilayer sheets [3]. M. A. Malik et. al. calculated the Zagreb indices in Titania nanotubes [8]. Recently, A. Ahmad et. al. computed the degree based topological indices of line graph of benzene ring [1]. Also, A. Raheem et. al. used M-Polynomials to calculate topological indices in Titania [6].

The graph of $TiO_2[m, n]$ nanotubes is shown in Figure 1 [9].

In the following article, for the sake of simplicity, wherever Titania nanotubes are mentioned, we mean the same as Titania nanotube $TiO_2[m, n]$.

4. Main Results

Given that in the graph of Titania nanotubes there are always $\delta(H) = 2$ and $\Delta(H) = 5$, so for each arbitrary vertex x, we have:

$$2 \leq d_x \leq 5.$$

There are four types of edges in Titania nanotubes:

$$\begin{aligned} e_1 &= \{(d_x, d_y) \mid uv \in E(H), d_x = 2, d_y = 4\}, \\ e_2 &= \{(d_x, d_y) \mid uv \in E(H), d_x = 2, d_y = 5\}, \\ e_3 &= \{(d_x, d_y) \mid uv \in E(H), d_x = 3, d_y = 4\}, \\ e_4 &= \{(d_x, d_y) \mid uv \in E(H), d_x = 3, d_y = 5\}. \end{aligned}$$

According to Figure 1 we have the following table for Titania nanotubes:

As a result, the number of edges of Titania nanotubes is equal to:

Table 1

Types and number of $TiO_2[m, n]$ edges

Edge type	Number of edges	$r_H(y)$	$r_H(x)$	ψ_i	ψ_i'	ψ_i''	ψ_i'''
e_1	$6m+2$	5	3	8	15	64	225
e_2	$4mn+2m+2$	5	2	7	10	49	100
e_3	$2m+2$	4	3	7	12	49	144
e_4	$6mn+6n-2m-2$	4	2	6	8	36	64

$$
\begin{aligned}
|E(TiO_2[m,n])| &= 6m+2+4mn+2m+2+2m+2+6mn+6n-2m-2 \\
&= 10mn+8m+6n+4.
\end{aligned}
$$

Theorem 1: *Suppose H is a graph of Titania nanotubes $TiO_2[m, n]$. Then we have,*

i) $R_1(H) = 64mn + 64m + 36n + 32$,

ii) $R_2(H) = 88mn + 118m + 48n + 72$.

Proof:

$$
\begin{aligned}
R_1(H) &= \sum_{i=1}^{|E(H)|} \psi_i = 8(6m+2)+7(4mn+2m+2) \\
&\quad +7(2m+2)+6(6mn+6n-2m-2) \\
&= 64mn+64m+36n+32.
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
R_2(H) &= \sum_{i=1}^{|E(H)|} \psi'_i = 15(6m+2)+10(4mn+2m+2) \\
&\quad +12(2m+2)+8(6mn+6n-2m-2) \\
&= 88mn+118m+48n+72.
\end{aligned}
$$

Theorem 2: *Suppose H is a graph of Titania nanotubes $TiO_2[m, n]$. Then we have,*

i) $HR_1(H) = 412mn + 508m + 216n + 252$,

ii) $HR_2(H) = 784mn + 1710m + 384n + 810$.

Proof:

$$
\begin{aligned}
HR_1(H) &= \sum_{i=1}^{|E(H)|} \psi''_i = 64(6m+2)+49(4mn+2m+2) \\
&\quad +49(2m+2)+36(6mn+6n-2m-2) \\
&= 412mn+508m+216n+252.
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
HR_2(H) &= \sum_{i=1}^{|E(H)|} \psi'''_i = 225(6m+2)+100(4mn+2m+2) \\
&\quad +144(2m+2)+64(6mn+6n-2m-2) \\
&= 784mn+1710m+384n+810.
\end{aligned}
$$

The line graph of the Titania nanotube is shown in Figure (2).
There are ten types of edges in Titania nanotubes:

$$e_1 = \{(d_x, d_y) \mid uv \in E(H), d_x = 2, d_y = 3\},$$
$$e_2 = \{(d_x, d_y) \mid uv \in E(H), d_x = 2, d_y = 5\},$$
$$e_3 = \{(d_x, d_y) \mid uv \in E(H), d_x = 3, d_y = 4\},$$
$$e_4 = \{(d_x, d_y) \mid uv \in E(H), d_x = 3, d_y = 6\},$$
$$e_5 = \{(d_x, d_y) \mid uv \in E(H), d_x = 4, d_y = 4\},$$
$$e_6 = \{(d_x, d_y) \mid uv \in E(H), d_x = 4, d_y = 5\},$$
$$e_7 = \{(d_x, d_y) \mid uv \in E(H), d_x = 4, d_y = 6\},$$
$$e_8 = \{(d_x, d_y) \mid uv \in E(H), d_x = 5, d_y = 5\},$$
$$e_9 = \{(d_x, d_y) \mid uv \in E(H), d_x = 5, d_y = 6\},$$
$$e_{10} = \{(d_x, d_y) \mid uv \in E(H), d_x = 6, d_y = 6\}.$$

As a result, the number of $L(TiO_2[m, n])$ edges is equal to:

$$\begin{aligned} E(L(TiO_2[m,n])) &= 2+2+8+2+8m+8n-6+8m+8n-4+4mn+4m \\ &\quad +24mn-10m+11mn-4m-5n \\ &= 39mn+6m+11n+4. \end{aligned}$$

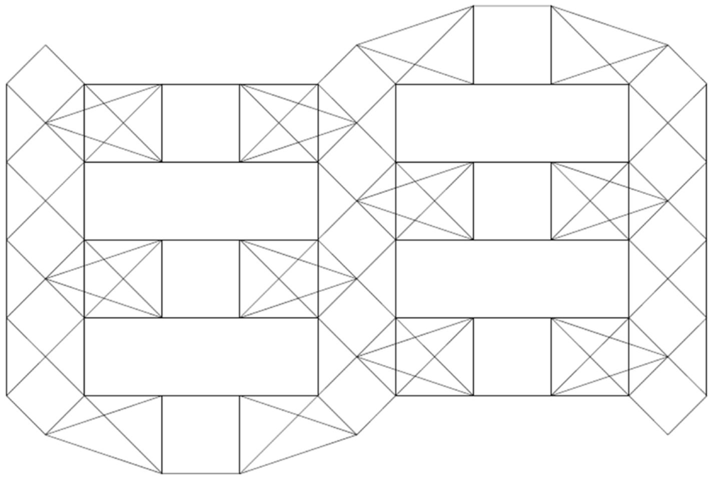

Figure 2

The line graph of Titania nanotube

According to Figure 2, we have the following table for the line graph:

Table 2

Types and number of edges in $L(TiO_2[m, n])$

Edge type	Number of edges	$r_H(y)$	$r_H(x)$	ψ_i	ψ_i'	ψ_i''	ψ_i'''
e_1	2	5	4	9	20	81	400
e_2	2	5	2	7	10	49	100
e_3	8	4	3	7	12	49	144
e_4	2	4	1	5	4	25	16
e_5	$8m+8n-6$	3	3	6	9	36	81
e_6	$8m$	3	2	5	6	25	36
e_7	$8n-4$	3	1	4	3	16	9
e_8	$4mn+4m$	2	2	4	4	16	16
e_9	$24mn-10m$	2	1	3	2	9	4
e_{10}	$11mn-4m-5n$	1	1	2	1	4	1

Theorem 3: *Suppose H is the line graph of the Titania nanotube. Then we have,*

i) $R_1(H) = 110mn + 66m + 70n + 46$,

ii) $R_2(H) = 75mn + 112m + 91n + 98$.

***Proof*:**

$$
\begin{aligned}
R_1(H) &= \sum_{i=1}^{|E(H)|} \psi_i = 9(2)+7(2)+7(8)+5(2)+6(8m+8n-6) \\
&\quad +5(8m)+4(8n-4)+4(4mn+4m)+3(24mn-10m) \\
&\quad +2(11mn-4m-5n) \\
&= 110mn+66m+70n+46.
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
R_2(H) &= \sum_{i=1}^{|E(H)|} \psi_i' = 20(2)+10(2)+12(8)+4(2)+9(8m+8n-6) \\
&\quad +6(8m)+3(8n-4)+4(4mn+4m)+2(24mn-10m) \\
&\quad +1(11mn-4m-5n) \\
&= 75mn+112m+91n+98.
\end{aligned}
$$

Theorem 4: *Suppose H is the line graph of the Titania nanotube. Then we have,*

i) $HR_1(H) = 171mn + 956m + 715n + 1662$,

ii) $HR_2(H) = 324mn + 446m + 396n + 422.$

***Proof*:**

$$\begin{aligned} HR_1(H) = \sum_{i=1}^{|E(H)|} \psi_i'' &= 400(2) + 100(2) + 144(8) + 16(2) + 81(8m + 8n - 6) \\ &+ 36(8m) + 9(8n - 4) + 16(4mn + 4m) + 4(24mn - 10m) \\ &+ 1(11mn - 4m - 5n) \\ &= 171mn + 956m + 715n + 1662. \end{aligned}$$

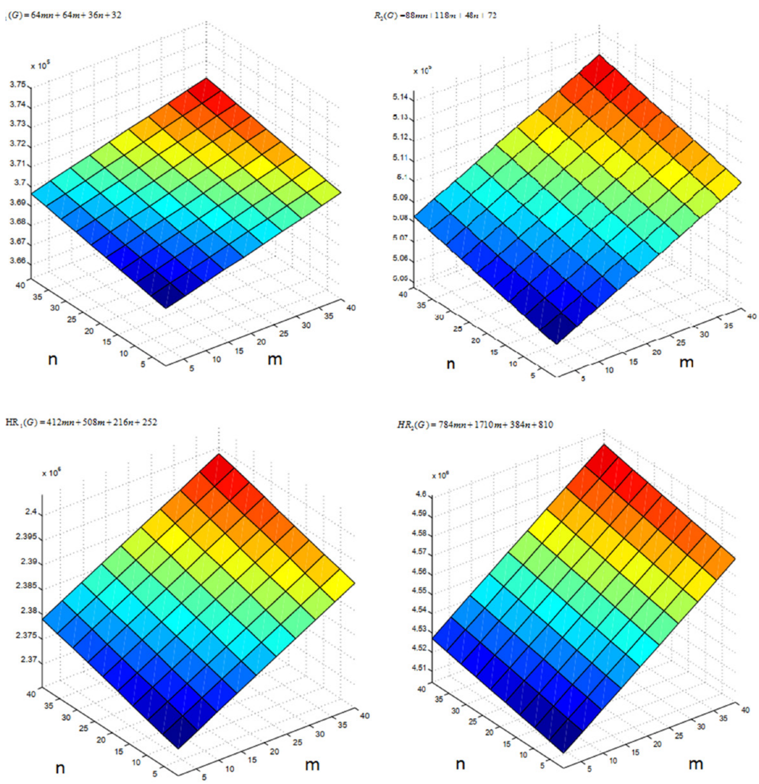

Figure 3

Graphs of Revan and Hyper Revan indices of Titania nanotubes using MAT-LAB

Similarly,

$$
\begin{aligned}
HR_2(H) = \sum_{i=1}^{|E(H)|} \psi_i''' &= 81(2) + 49(2) + 49(8) + 25(2) + 36(8m + 8n - 6) \\
&+25(8m) + 16(8n - 4) + 16(4mn + 4m) + 9(24mn - 10m) \\
&+ 4(11mn - 4m - 5n) \\
&= 324mn + 446m + 396n + 422.
\end{aligned}
$$

Finally, the diagrams obtained from drawing Revan and Hyper Revan indices, which are illustrated for Titania nanotubes with the help of MATLAB software version 13, which is illustrated in windows7 operating system with CPU: 2.3GHz.

Examining Figure 3, it is clear that the level of the second index of Revan is higher than the level of the first index of Revan. Also, the second index of Hyper Revan is at a higher level than the first index of Hyper Revan.

The second Revan index has the highest, and the first Hyper Revan index has the lowest level among these four charts.

5. Conclusion

In this article, a method for calculating Revan indices and Hyper Revan indices for Titanium nanotubes $TiO_2[m, n]$ is presented.

The advantage of these methods is that it makes the calculation of Revan indices much easier with the help of mathematical software. These indices were also expressed for $TiO_2[m, n]$. This method can also be used for other nanotubes.

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