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Computing K Banhatti and K Hyper Banhatti indices of Titania nanotubes $TiO_2[m, n]$

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Abstract

Graph theory has been used for modeling in chemistry. 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, by providing a method to obtain the degree of vertices in the section of the corresponding nanotube, the K Banhatti and K Hyper Banhatti indices are computing. Next, the K Banhatti and K Hyper Banhatti indices in the line graph of Titania nanotubes $TiO_2[m, n]$ are also computing. To compare the obtained values, diagrams of K Banhatti and K Hyper Banhatti indices are drawn.

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

Keywords: *K Banhatti indices, K Hyper Banhatti indices, Titania nanotubes, Line graph.*

1. Introduction

Numerical calculations are of particular importance in nanoscale simulations. Study in nanoscale leads to drastic changes in material properties. In nanoscience, the analysis 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 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.

In 1947, the first and most studied topological index was introduced by Weiner [9]. One of the practical tools in studying the structure and properties of a molecule, such as boiling point, evaporation heat, formation heat, chromatographic storage times, surface tension, vapor pressure, etc [4].

In this article, the Banhatti indices in the graph and line graph of Titania nanotubes are investigated.

2. Preliminaries

This section provides some of the required definitions. Suppose $G = (V, E)$ is a simple and connected graph. We represent the set of edges with $E(G)$ and the number of edges with $|E(G)|$ and the set of vertices with $V(G)$ and the number of vertices with $|V(G)|$. We denote the degree of vertex u by d_u and if there is an edge between two vertices u and v, represented it by $uv \in E(G)$.

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, K Banhatti and K Hyper Banhatti indices for graph G were introduced by V.R. Kulli in 2016 [7].

Definition 2.1: The first and second K Banhatti indices for graph G are defined as:

$$B_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)],$$

$$B_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

Which can be defined as $\psi_i = [d_G(u) + d_G(v)]$ by defining $B_1(G) = \sum_{i=1}^{|E(G)|} \psi_i$ and $\psi_i' = d_G(u) d_G(v)$ can also define $B_2(G) = \sum_{i=1}^{|E(G)|} \psi_i'$.

Definition 2.2: The first and second K Hyper Banhatti indices for graph G are defined as:

$$HB_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^2,$$
$$HB_2(G) = \sum_{uv \in E(G)} (d_G(u) d_G(v))^2.$$

Which can be defined as $\psi_i'' = [d_G(u) + d_G(v)]^2$ by defining $HB_1(G) = \sum_{i=1}^{|E(G)|} \psi_i''$ and $\psi_i''' = (d_G(u) d_G(v))^2$ can also define $HB_2(G) = \sum_{i=1}^{|E(G)|} \psi_i'''$.

Definition 2.3: In a non-empty graph *G*, 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 *G*, the resulting graph is denoted by *L*(*G*) and is called the line graph of *G* [1].

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

In this section, the structure of the Titania nanotube $TiO_2[m, n]$ is studied to compute the K Banhatti and K Hyper Banhatti 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 [10].

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].

Comprehensive theoretical studies on Titania nanotubes and their growth have not been clearly stated, so this issue has caused a great deal of interest and attention to studies in this field.

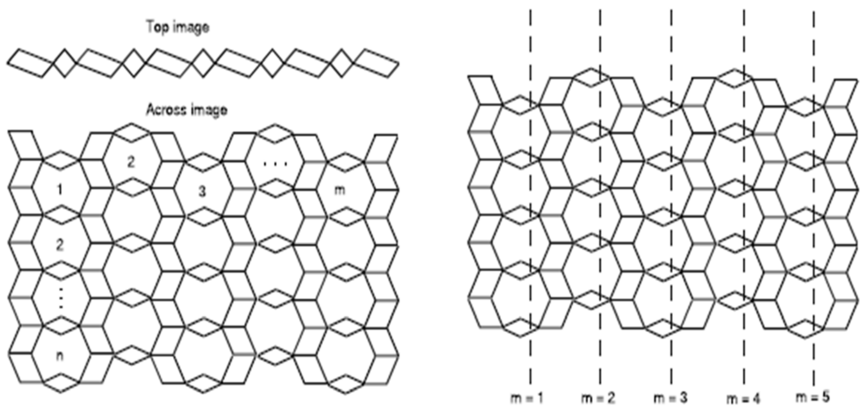

Figure 1

Nanotube $TiO_2[m, n]$

One of the characteristics of Titania nanotube sheets is the considerable stability of its atomic multilayer sheets [3].

Recently, M. A. Malik et. al. calculated the Zagreb indices in Titania nanotubes [8].

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, where m represents the number of octagons in a row and n represents the number of octagons in a column of Titania nanotubes.

In the following, 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 $\delta(G) = 2$ and $\Delta(G) = 5$, so for each arbitrary vertex u, we have:

$$2 \le d_u \le 5.$$

There are four types of edges in Titania nanotubes:

$$e_1 = \{(d_u, d_v) \mid uv \in E(G), d_u = 2, d_v = 4\},$$
$$e_2 = \{(d_u, d_v) \mid uv \in E(G), d_u = 2, d_v = 5\},$$
$$e_3 = \{(d_u, d_v) \mid uv \in E(G), d_u = 3, d_v = 4\},$$
$$e_4 = \{(d_u, d_v) \mid uv \in E(G), d_u = 3, d_v = 5\}.$$

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:

$$|E(TiO_2[m,n])| = 6m + 2 + 4mn + 2m + 2 + 2m + 2 + 6mn + 6n - 2m - 2$$
$$= 10mn + 8m + 6n + 4.$$

Table 1

Number of edges and edge type of $TiO_2[m, n]$

Number of edges	$d_G(u)$	$d_G(v)$	ψ_i	ψ_i'	ψ_i''	ψ_i'''	Edge type
$6m+2$	2	4	6	8	36	64	e_1
$4mn+2m+2$	2	5	7	10	49	100	e_2
$2m+2$	3	4	7	12	49	144	e_3
$6mn+6n-2m-2$	3	5	8	15	25	225	e_4

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

i) $B_1(G) = 76mn + 48m + 48n + 24$,

ii) $B_2(G) = 130mn + 62m + 90n + 30$.

***Proof*:**

$$\begin{aligned} B_1(G') = \sum_{i=1}^{|E(G)|} \psi_i &= 9(2) + 7(2) + 7(8) + 5(2) + 6(8m + 8n - 6) \\ &+ 5(8m) + 4(8n - 4) + 4(4mn + 4m) + 3(24mn - 10m) \\ &+ 2(11mn - 4m - 5n) \\ &= 110mn + 66m + 70n + 46. \end{aligned}$$

Similarly, we have,

$$\begin{aligned} B_2(G) = \sum_{i=1}^{|E(G)|} \psi'_i &= 8(6m + 2) + 10(4mn + 2m + 2) + 12(2m + 2) \\ &+ 15(6mn + 6n - 2m - 2) \\ &= 130mn + 62m + 90n + 30. \end{aligned}$$

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

i) $HB_1(G) = 346mn + 362m + 150n + 218$,

ii) $HB_2(G) = 1750mn + 422m + 1350n + 166$.

***Proof*:**

$$\begin{aligned} HB_1(G) = \sum_{i=1}^{|E(G)|} \psi''_i &= 36(6m + 2) + 49(4mn + 2m + 2) + 49(2m + 2) \\ &+ 25(6mn + 6n - 2m - 2) \\ &= 346mn + 362m + 150n + 218. \end{aligned}$$

Similarly, we have,

$$\begin{aligned} HB_2(G) = \sum_{i=1}^{|E(G)|} \psi'''_i &= 64(6m + 2) + 100(4mn + 2m + 2) + 144(2m + 2) \\ &+ 225(6mn + 6n - 2m - 2) \\ &= 1750mn + 422m + 1350n + 166. \end{aligned}$$

The line graph of the Titania nanotube is shown in Figure 2.

There are ten types of edges in Titania nanotubes:

$$
\begin{aligned}
e_1 &= \{(d_u, d_v) \mid uv \in E(G), d_u = 2, d_v = 3\},\\
e_2 &= \{(d_u, d_v) \mid uv \in E(G), d_u = 2, d_v = 5\},\\
e_3 &= \{(d_u, d_v) \mid uv \in E(G), d_u = 3, d_v = 4\},\\
e_4 &= \{(d_u, d_v) \mid uv \in E(G), d_u = 3, d_v = 6\},\\
e_5 &= \{(d_u, d_v) \mid uv \in E(G), d_u = 4, d_v = 4\},\\
e_6 &= \{(d_u, d_v) \mid uv \in E(G), d_u = 4, d_v = 5\},\\
e_7 &= \{(d_u, d_v) \mid uv \in E(G), d_u = 4, d_v = 6\},\\
e_8 &= \{(d_u, d_v) \mid uv \in E(G), d_u = 5, d_v = 5\},\\
e_9 &= \{(d_u, d_v) \mid uv \in E(G), d_u = 5, d_v = 6\},\\
e_{10} &= \{(d_u, d_v) \mid uv \in E(G), d_u = 6, d_v = 6\}.
\end{aligned}
$$

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

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

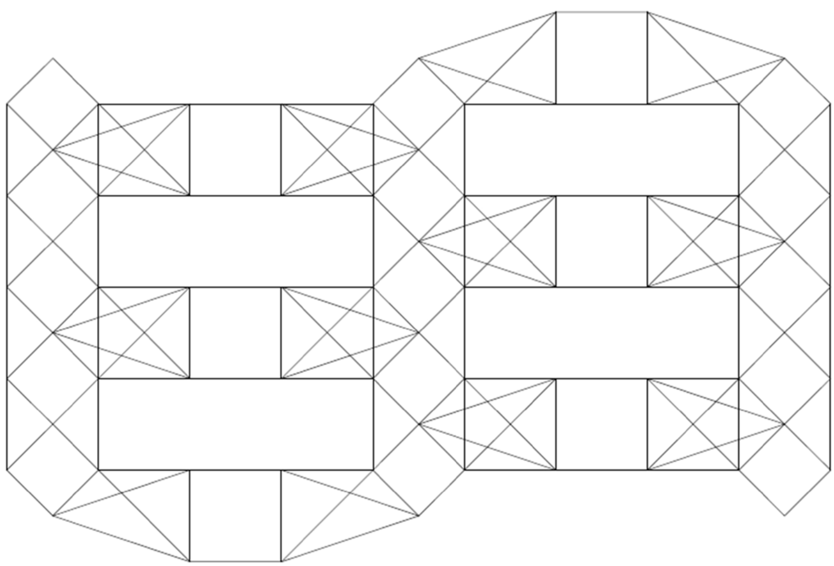

Figure 2

***L*(*TiO*$_2$[*m*, *n*])**

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

Table 2

Number of edges and edge type of $L(TiO_2[m, n])$

Number of edges	$d_G(u)$	$d_G(v)$	ψ_i	ψ_i'	ψ_i''	ψ_i'''	Edge type
2	2	3	5	6	25	36	e_1
2	2	5	7	10	49	100	e_2
8	3	4	7	12	49	144	e_3
2	3	6	9	18	81	324	e_4
$8m$+$8n$-6	4	4	8	16	64	256	e_5
$8m$	4	5	9	20	81	400	e_6
$8n$-4	4	6	10	24	100	576	e_7
$4mn$+$4m$	5	5	10	25	100	625	e_8
$24mn$-$10m$	5	6	11	30	121	900	e_9
$11mn$-$4m$-$5n$	6	6	12	36	144	1296	e_{10}

Theorem 3: *Suppose G' is the line graph of the Titania nanotube, then we have,*

i) $B_1(G') = 436mn + 18m + 84n + 10$,

ii) $B_2(G') = 1216mn - 56m + 140n - 28.$

***Proof*:**

$$\begin{aligned} B_1(G') = \sum_{i=1}^{|E(G)|} \psi_i &= 5(2)+7(2)+7(8)+9(2)+8(8m+8n-6) \\ &+9(8m)+10(8n-4)+10(4mn+4m)+11(24mn-10m) \\ &+12(11mn-4m-5n) \\ &= 436mn+18m+84n+10. \end{aligned}$$

Similarly, we have,

$$\begin{aligned} B_2(G') = \sum_{i=1}^{|E(G)|} \psi_i' &= 6(2)+10(2)+12(8)+18(2)+16(8m+8n-6) \\ &+20(8m)+24(8n-4)+25(4mn+4m)+30(24mn-10m) \\ &+36(11mn-4m-5n) \\ &= 1216mn-56m+140n-28. \end{aligned}$$

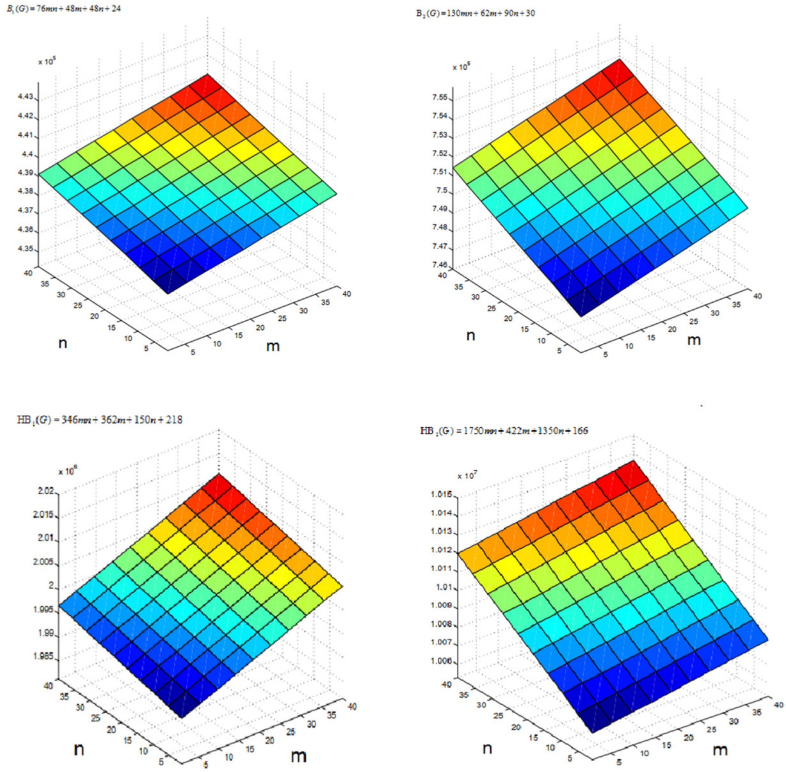

Figure 3

Graphs of K Banhatti and K Hyper Banhatti indices of $TiO_2[m, n]$ using MATLAB.

Theorem 4: Suppose G' is the line graph of the Titania nanotube, then we have,

i) $HB_1(G') = 4888mn - 226m + 592n - 82$,

ii) $HB_2(G') = 38356mn - 6436m + 176n - 1768$.

***Proof*:**

$$\begin{aligned} HB_1(G') = \sum_{i=1}^{|E(G)|} \psi_i'' &= 25(2) + 49(2) + 49(8) + 81(2) + 64(8m + 8n - 6) \\ &+ 81(8m) + 100(8n - 4) + 100(4mn + 4m) \\ &+ 121(24mn - 10m) + 144(11mn - 4m - 5n) \\ &= 4888mn - 226m + 592n - 82. \end{aligned}$$

Similarly, we have,

$$
\begin{aligned}
HB_2(G') = \sum_{i=1}^{|E(G)|} \psi_i'''' &= 36(2)+100(2)+144(8)+324(2) \\
&+256(8m+8n-6)+400(8m)+576(8n-4) \\
&+625(4mn+4m)+900(24mn-10m) \\
&+1296(11mn-4m-5n) \\
&= 38356mn-6436m+176n-1768.
\end{aligned}
$$

Finally, the diagrams obtained from drawing K Banhatti and K Hyper Banhatti indices, which are illustrated for Titania nanotubes with the help of MATLAB software.

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

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

5. Conclusion

In this article, a method for computing K Banhatti and K Hyper Banhatti indices for Titania nanotubes $TiO_2[m, n]$ is presented.

The advantage of these methods is that it makes the computing of K Banhatti 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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