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COMPUTATIONS OF CERTAIN TOPOLOGICAL INDICES OF TITANIA NANOTUBES $TiO_2(m, n)$

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Abstract: A *topological index* is a numeric quantity associated with a graph which characterizes the topology of graph and is invariant under graph automorphism. The *third geometric-arithmetic index (GA_3)* of a graph G is defined as
$GA_3(G) = \sum_{e=uv\in E(G)} \frac{2\sqrt{m_v.m_u}}{m_v+m_u}$. In this paper, we compute the third version of geometric-arithmetic index of the *Titania Nanotubes* $TiO_2(m,n)$.

AMS Subject Classification: 05C90, 05C35, 05C12
Key Words: molecular graph, titania carbon nanotubes $TiO_2(m,n)$, orthogonal cuts, geometric-arithmetic index

1. Introduction

Mathematical chemistry is the branch of theoretical chemistry in which we discuss and predict the behavior of mathematical structure by using mathematical tools. There are numerous of topological indices that have found some applications in theoretical chemistry, especially in QSPR/QSAR research.

Throughout this paper we consider a simple connected a graph and with $V(G)$ be the set of vertices represents the atoms and $E(G)$ the set of edges corresponds to the chemical bonds. For two vertices u and v, uv is defined to be an edge and are said to be connected the set of all vertices connected to u is called the neighborhood of u denoted by $N(u)$. The total number of such connected edges represents the degree of the vertex u. The length of the shortest path between two vertices is called the topological distance and is denoted by $d(u,v)$, the maximum distance between the vertex u and any vertex v in G is named the eccentricity of u and is denoted $ecc(u)$.

I. Gutman [23] introduced a new topological index after the Wiener index, and named it the *Szeged Index.* Suppose there is an $e = uv \in E(G)$ connecting the vertices u and v defines:

$$m_u(e|G) = \{x|x \in E(G), d(u,x) < d(x,v)\},$$

$$m_v(e|G) = \{x|x \in E(G), d(v,x) < d(x,u)\},$$

where $m_u(e|G)$ is the number of edges of G lying near to u than to v and $m_v(e|G)$ is the number of edges of G lying near to v than to u, thus the version Szeged index of a graph G is defined as:

$$Sz_v(G) = \sum_{e\in E(G)} [n_u(e|G) \times n_v(e|G)],$$

The edge version of Szeged index introduced recently by *I. Gutman* and *A.R. Ashrafi* [21] and was computed for some graphs [21, 24]. Readers are encouraged to see [27, 2, 1, 22, 25, 26, 5, 4] for computations of this index for some graph.

$$Sz_e(G) = \sum_{e \in E(G)} [m_u(e|G) \times m_v(e|G)],$$

The Geometric arithmetic GA index was introduced in [31] and is defined as:

$$GA = \sum \frac{2\sqrt{d_u.d_v}}{d_u + d_v}$$

TiO_2 is one of the most studied compounds in materials science. Owing to some outstanding properties it is used for instance in photo catalysis, dye-sensitized solar cells, and biomedical devices. Now we compute third geometric arithmetic index of Titania Nanotubes which is our main result.

2. Main Result and Discussion

Consider Titania Nanotubes $TiO_2(m, n)$ for all $m, n \in N$ depicted in Fig.1. This graph has $2(3n + 2)(m + 1)$ vertices and $10mn + 6m + 8n + 4$ edges. This graph has $2mn + 4n + 4$ vertices of degree two, $2n$ vertices of degree four, $2mn$ vertices with degree five and the vertices of degree three are $2mn + 4m$(Se the paper series [3],[6],[7]-[13].

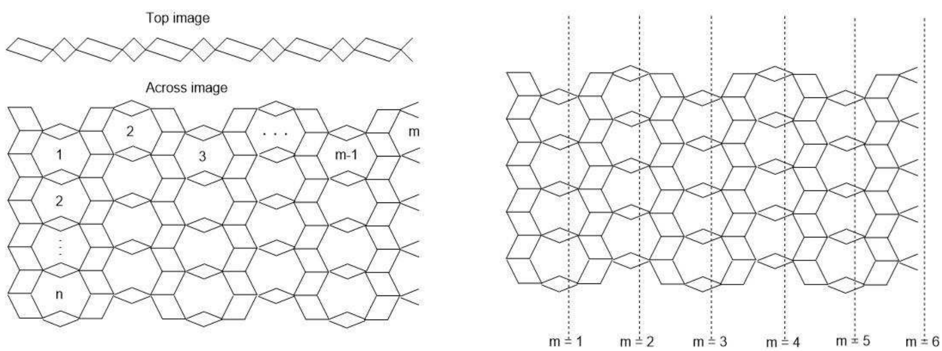

Figure 1. [15] A graphical representation of Titania Nanotubes *TiO_2[m,n].*

By taking the orthogonal cuts of the graph, we obtain the number of edges in the left component representing $m_u(e|TiO_2(m, n))$ and the number of edges in the right component as $m_v(e|TiO_2(m,n))$ with $5n+3$ vertical cuts for horizontal edges. Now e being an oblique edge we denote its orthogonal cut by C_i or F_j $\forall i = 1, 2, \cdots, 2(n+1)$ and $j = 1, \cdots, 3n+1$.

Note that the size of all orthogonal cuts is equivalent with $|C_i| = 2m+1$ and $|F_i| = 2(m+1)$.

In the case of orthogonal cuts C_i $(i = 1, \cdots, 2(n+1))$, see Figure 2:

- For C_1: $m_u(e_1|TiO_2(m,n)) = 0$ and $m_v(e_1|TiO_2(m,n)) = |E(TiO_2(m,n)| - |C_1| = 10mn + 6m + 8n + 4 - (2m+1) = 10mn + 4m + 8n + 3$.
- For C_2: $m_u(e_2|TiO_2(m,n)) = |C_1| + |F_1| = 2m+1+2m+2 = 4m+3$ and $m_v(e_2|TiO_2(m,n)) = |E(TiO_2(m,n))| - (|C_1| + |F_1| + |C_2|) = 10mn + 6m + 8n + 4 - (6m+4) = 10mn + 2m + 8n$.
- For C_3: $m_u(e_3|TiO_2(m,n)) = 2|C_1| + 3|F_1| = 10m+8$ and $m_v(e_3|TiO_2(m,n)) = |E(TiO_2(m,n)| - (3|C_1| + 3|F_1|) = 10mn + 6m + 8n + 4 - (12m+9) = 10mn + 8n - 6m - 5$.
- For C_4: $m_u(e_4|TiO_2(m,n)) = 3|C_1| + 4|F_1| = 14m+11$ and $m_v(e_4|TiO_2(m,n)) = |E(TiO_2(m,n)| - (3|C_1| + 4|F_1|) = 10mn + 6m + 8n + 4 - (16m+12) = 10mn + 8n - 10m - 8$.
- For C_{2h-1}: $m_u(e_{2h-1}|TiO_2(m,n)) = (2h-2)|C_1| + (3h-3)|F_1| = (2h-2)(2m+1) + (3h-3)(2m+2) = (10m+8)(h-1)$ and $m_v(e_{(2h-1)}|TiO_2(m,n)) = |E(TiO_2(m,n)| - ((2h-1)|C_1| + (3h-3)|F_1|) = 10mn + 6m + 8n + 4 - (10m+8)(h-1) - (2m+1)$.
- For C_{2h}: $m_u(e_{2h}|TiO_2(m,n)) = (2h-1)|C_1| + (3h-2)|F_1| = (2h-1)(2m+1) + (3h-2)(2m+2) = 10hm + 8h - 6m - 5$ and $m_v(e_{2h}|TiO_2(m,n)) = |E(TiO_2(m,n)| - (2h|C_1| + (3h-1)|F_1|) = 10m(n-h) + 10m + 8(n-h) + 8$.
- For C_{2n+2}: $m_u(e_{2n+2}|TiO_2(m,n)) = (2n+1)|C_1| + (3n+1)|F_1| = (2h-1)(2m+1) + (3h-2)(2m+2) = 10nm + 8n + 4m + 3$ and $m_v(e_{2n+2}|TiO_2(m,n)) = 0$.

In the case of orthogonal cuts $F_j (j = 1, \ldots, 3n+1)$, see Figure 2:

- For F_1: $m_u(e_1|TiO_2(m,n)) = 2m+1 = |C_i|$ and $m_v(e_1|TiO2(m,n) = |E(TiO_2(m,n)| - (|C_1| + |F_1|) = 10mn + 6m + 8n + 4 - (4m+3) = 10mn + 8n + 2m + 1$.
- For F_2: $m_u(e_2|TiO_2(m,n)) = 2|C_1| + |F_1| = 6m+4$ and $m_v(e_2|TiO_2(m,n) = |E(TiO2(m,n)| - (2|C_1| + 2|F_1|) = 10mn + 6m + 8n + 4 - (8m+6) = 10mn + 8n - 2m - 2$.
- For F_3: $m_u(e_3|TiO_2(m,n)) = 2|C_1| + 2|F_1| = 8m+6$ and $m_v(e_3|TiO_2(m,n) = |E(TiO2(m,n)| - (2|C_1| + 3|F_1|) = 10mn + 6m + 8n + 4 - (10m+8) = 10mn + 8n - 4m - 4$.
- For F_4: $m_u(e_4|TiO_2(m,n)) = 3|C_1| + 3|F_1| = 12m+9$ and $m_v(e_4|TiO_2(m,n) = |E(TiO2(m,n)| - (3|C_1| + 4|F_1|) = 10mn + 6m + 8n + 4 - (14m+11) = 10mn + 8n - 8m - 7$.

• For F_5: $m_u(e_5|TiO_2(m,n)) = 4|C_1|+4|F_1| = 16m+12$ and $m_v(e_5|TiO_2(m,n) = |E(TiO2(m,n)| - (4|C_1| + 5|F_1|) = 10mn + 6m + 8n + 4 - (18m + 14) = 10mn + 8n - 12m - 10$.
• For F_6: $m_u(e_6|TiO_2(m,n)) = 4|C_1|+5|F_1| = 18m+13$ and $m_v(e_6|TiO_2(m,n) = |E(TiO2(m,n)| - (4|C_1| + 6|F_1|) = 10mn + 6m + 8n + 4 - (20m + 15) = 10mn + 8n - 14m - 11$.
• For F_7: $m_u(e_7|TiO_2(m,n)) = 5|C_1|+6|F_1| = 22m+17$ and $m_v(e_7|TiO_2(m,n) = |E(TiO2(m,n)| - (4|C_1| + 6|F_1|) = 10mn + 6m + 8n + 4 - (24m + 19)$.
• For F_8: $m_u(e_8|TiO_2(m,n)) = 6|C_1|+7|F_1| = 22m+17$ and $m_v(e_8|TiO_2(m,n) = |E(TiO2(m,n)| - (4|C_1| + 6|F_1|) = 10mn + 6m + 8n + 4 - (24m + 19)$.
• For $F_{3h+1}(h = 0,\ldots,n)$: $m_u(F_{3h+1}|TiO_2(m,n)) = (2h+1)|C_1| + (3h)|F_1| = (2h+1)(2m+1)+(3h)(2m+2) = 10hm+2m+8h+1$ and $m_v(F_{3h+1}|TiO_2(m,n)) = |E(TiO_2(m,n)| - (10hm + 4m + 8h + 3) = (10m + 8)(n - h) + 2m + 1$.
• For $F_{3h-1}(h = 1,\ldots,n)$: $m_u(F_{3h-1}|TiO_2(m,n)) = (2h)|C_1| + (3h-2)|F_1| = (2h)(2m + 1) + (3h - 2)(2m + 2) = (10m + 8)h - 2|F_1| = 10hm - 4m + 8h - 4$ and $m_v(F_{3h-1}|TiO2(m,n)) = (10mn+6m+8n+4) - (10hm - 2m + 8h - 2) = (10m + 8)(n - h) + 8m + 6$.
• For $F_{3h}(h = 1,\ldots,n)$: $m_u(F_{3h}|TiO2(m,n)) = m_u(F_{3h-1}|TiO_2(m,n))+|F_1| = 2h|C_1| + (3h - 1)|F_1| = (10m + 8)h - 2m - 2$ and $m_v(F_{3h}|TiO_2(m,n)) = m_v(F_{3h-1}|TiO_2(m,n)) - |F_1| = (10m + 8)(n - h) + 6m + 4$.
Based on the above calculations we have two following results.

Theorem 1. *The third geometric-arithmetic index (GA_3) of Titania Nanotubes $TiO_2[m,n]$ is equal to*

$$\begin{aligned} GA_3(TiO_2[m,n]) =& \frac{2(2m+1)}{10mn+4m+8n+3} \\ &\times \sum_{h=1}^{n+1} \Big[\sqrt{2(5m+4)(h-1)((10m+8)(n-h)+14m+11)} \\ &+ \sqrt{2(10hm+8h-6m-5)(5m+4)(n-h+1)} \Big] \\ &+ \frac{2(m+1)}{5mn+2m+4n+1} \\ &\times \sum_{k=1}^{n} \Big[\sqrt{(10mk+8k+2m+1)((10m+8)(n-k)+2m+1)} \\ &+ 2\sqrt{(5mk+4k-m-1)((5m+4)(n-k)+3m+2)} \\ &+ 2\sqrt{(5mk+4k-2m-2)((5m+4)(n-k)+4m+3)} \Big] \end{aligned}$$

$$+\frac{2(m+1)\sqrt{(2m+1)(10mn+8n+2m+1)}}{5mn+2m+4n+1}$$

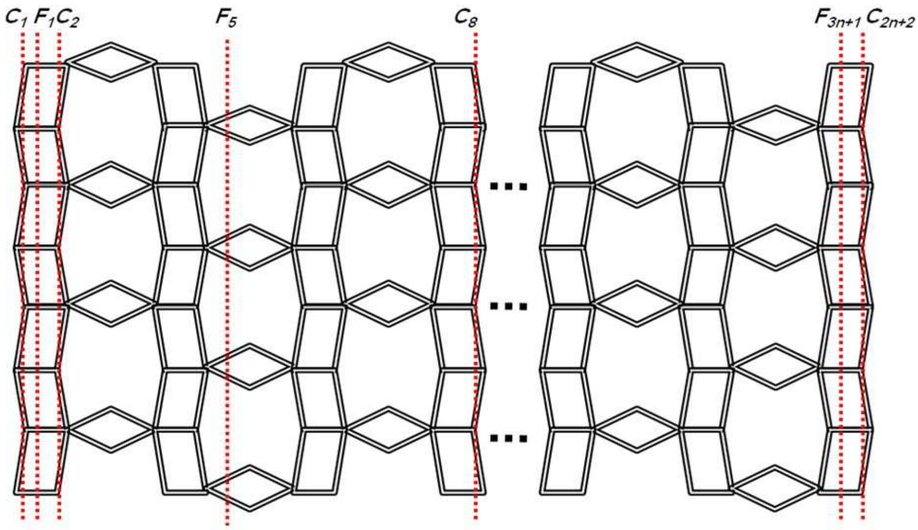

Figure 2. *[3, 29, 30, 6, 15] Orthogonal cuts representation of the Titania Nanotubes.*

Proof. From the definition of third geometric arithmetic index and the above calculation we have

$$GA_3(TiO_2[m,n]) = \sum_{e_i=uv\in E(TiO_2(m,n))} \frac{2\sqrt{m_v.m_u}}{m_v+m_u}$$

$$= \sum_{e_i=uv\in C_i\ ,\ i=1,\cdots,2n+2} |C_i|\Big[\frac{2\sqrt{m_v(e_i|(TiO_2(m,n)).m_u(e_i|(TiO_2(m,n))}}{m_v(e_i|(TiO_2(m,n))+m_u(e_i|(TiO_2(m,n))}\Big]$$

$$+\sum_{f_i=uv\in F_i\ ,\ i=1,\cdots,3n+1} |F_i|\Big[\frac{2\sqrt{m_v(f_i|(TiO_2(m,n)).m_u(f_i|(TiO_2(m,n))}}{m_v(f_i|(TiO_2(m,n))+m_u(f_i|(TiO_2(m,n))}\Big]$$

$$=|C_1|\sum_{e_{2h-1}=vu\in C_{2h-1}\ ,\ h=1,\cdots,n+1}\Big[\frac{2\sqrt{m_v(e_{2h-1}|(TiO_2(m,n)).m_{2h-1}(e_i|(TiO_2(m,n))}}{m_v(e_{2h-1}|(TiO_2(m,n))+m_{2h-1}(e_i|(TiO_2(m,n))}\Big]$$

$$+|C_1|\sum_{e_{2h-1}=vu\in C_{2h}\ ,\ h=1,\cdots,n+1}\Big[\frac{2\sqrt{m_v(e_{2h}|(TiO_2(m,n)).m_{2h}(e_i|(TiO_2(m,n))}}{m_v(e_{2h}|(TiO_2(m,n))+m_{2h}(e_i|(TiO_2(m,n))}\Big]$$

$$+|F_1|\sum_{f_{3h-1}=vu\in F_{3k+1}\ ,\ k=0,\cdots,n}\Big[\frac{2\sqrt{m_v(f_{3k+1}|(TiO_2(m,n)).m_{2h}(f_{3k+1}|(TiO_2(m,n))}}{m_v(f_{3k+1}|(TiO_2(m,n))+m_{2h}(f_{3k+1}|(TiO_2(m,n))}\Big]$$

$$+|F_1|\sum_{f_{3h}=vu\in F_{3k}\ ,\ k=1,\cdots,n}\Big[\frac{2\sqrt{m_v(f_{3k}|(TiO_2(m,n)).m_{2h}(f_{3k}|(TiO_2(m,n))}}{m_v(f_{3k}|(TiO_2(m,n))+m_{2h}(f_{3k}|(TiO_2(m,n))}\Big]$$

$$+|F_1| \sum_{f_{3h-1}=vu\in F_{3k-1}\ ,\ k=1,\cdots,n} \Big[\frac{2\sqrt{m_v(f_{3k-1}|(TiO_2(m,n)).m_{2h}(f_{3k-1}|(TiO_2(m,n))}}{m_v(f_{3k-1}|(TiO_2(m,n))+m_{2h}(f_{3k-1}|(TiO_2(m,n))}\Big]$$

$$=(2m{+}1)\sum_{e_{2h-1}=vu\in C_{2h-1}\ ,\ h=1,\cdots,n+1}\Big[\frac{2\sqrt{(10m+8)(h-1)\times((10mn+8n+6m+4)-(10m+8)(h-1)-(2m+1))}}{(10m+8)(h-1)+(10mn+8n+6m+4)-(10m+8)(h-1)-(2m+1)}\Big]$$

$$+(2m+1)\sum_{e_{2h-1}=vu\in C_{2h}\ ,\ h=1,\cdots,n+1}\Big[\frac{2\sqrt{(10hm+8h-6m-5)\times(10m(n-h)+10m+8(n-h)+8)}}{(10hm+8h-6m-5)+(10m(n-h)+10m+8(n-h)+8)}\Big]$$

$$+2(m+1)\sum_{f_{3h-1}=vu\in F_{3k+1}\ ,\ h=0,\cdots,n}\Big[\frac{2\sqrt{(10hm+2m+8h+1)\times((10m+8)(n-h)+2m+1)}}{(10hm+2m+8h+1)+((10m+8)(n-h)+2m+1)}\Big]$$

$$+2(m+1)\sum_{f_{3h}=vu\in F_{3k}\ ,\ h=1,\cdots,n}\Big[\frac{2\sqrt{((10m+8)h-2m-2)\times((10m+8)(n-h)+6m+4)}}{((10m+8)h-2m-2)+((10m+8)(n-h)+6m+4)}\Big]$$

$$+2(m+1)\sum_{f_{3h-1}=vu\in F_{3k-1}\ ,\ h=1,\cdots,n}\Big[\frac{2\sqrt{(10hm-4m+8h-4)\times((10m+8)(n-h)+8m+6)}}{(10hm-4m+8h-4)+((10m+8)(n-h)+8m+6)}\Big]$$

$$=(2m+1)\sum_{e_{2h-1}=vu\in C_{2h-1}\ ,\ h=1,\cdots,n+1}\Big[\frac{2\sqrt{(10mh+8h-10m-8)\times(10mn-10mh-8h+14m+8n+11)}}{10mn+4m+8n+3}\Big]$$

$$+(2m+1)\sum_{e_{2h-1}=vu\in C_{2h}\ ,\ h=1,\cdots,n+1}\Big[\frac{2\sqrt{(10hm+8h-6m-5)\times(10mn-10mh-8h+10m+8n+8)}}{10mn+4m+8n+3}\Big]$$

$$+2(m+1)\sum_{f_{3h-1}=vu\in F_{3k+1}\ ,\ h=0,\cdots,n}\Big[\frac{2\sqrt{(10hm+2m+8h+1)\times(10mn-10mh+8n-8h+2m+1)}}{(10mn+4m+8n+2)}\Big]$$

$$+2(m+1)\sum_{f_{3h}=vu\in F_{3k}\ ,\ h=1,\cdots,n}\Big[\frac{2\sqrt{(10mh+8h-2m-2)(10mn-10mh+8n-8h+6m+4)}}{(10mn+4m+8n+2)}\Big]$$

$$+2(m+1)\sum_{f_{3h-1}=vu\in F_{3k-1}\ ,\ h=1,\cdots,n}\Big[\frac{2\sqrt{(10hm-4m+8h-4)\times(10mn-10mh+8n-8h+8m+6)}}{(10mn+4m+8n+2)}\Big]$$

$$=\frac{2(2m+1)}{10mn+4m+8n+3}\sum_{h=1}^{n+1}\Big[\sqrt{(10mh+8h-10m-8)(10mn-10mh-8h+14m+8n+11)}$$

$$+\sqrt{(10hm+8h-6m-5)(10mn-10mh-8h+10m+8n+8)}\Big]$$

$$+\frac{2(m+1)}{5mn+2m+4n+1}\sum_{h=1}^{n}\Big[\sqrt{(10hm+2m+8h+1)(10mn-10mh+8n-8h+2m+1)}$$

$$+\sqrt{(10mh+8h-2m-2)(10mn-10mh+8n-8h+6m+4)}+\sqrt{(10hm-4m+8h-4)(10mn-10mh+8n-8h+8m+6)}\Big]$$

$$+\frac{2(m+1)\times 2\sqrt{(2m+1)(10mn+8n+2m+1)}}{10mn+4m+8n+2}$$

$$=\frac{2(2m+1)}{10mn+4m+8n+3}\sum_{h=1}^{n+1}\Big[\sqrt{2(5mh+4h-5m-4)(10m(n-h)+8(n-h)+14m+11)}$$

$$+\sqrt{2(10hm+8h-6m-5)(5m(n-h)+4(n-h)+5m+4)}\Big]$$

$$+\frac{2(m+1)}{5mn+2m+4n+1}\sum_{h=1}^{n}\Big[\sqrt{(10hm+2m+8h+1)(10m(n-h)+8(n-h)+2m+1)}$$

$$+2\sqrt{(5mh+4h-m-1)(5m(n-h)+4(n-h)+3m+2)}$$

$$+2\sqrt{(5hm+4h-2m-2)(5m(n-h)+4(n-h)+4m+3)}\Big]$$

$$
\begin{aligned}
&+\frac{2(m+1)\sqrt{(2m+1)(10mn+8n+2m+1)}}{5mn+2m+4n+1}\\
=&\frac{2(2m+1)}{10mn+4m+8n+3}\sum_{h=1}^{n+1}\Big[\sqrt{2(5m+4)(h-1)((10m+8)(n-h)+14m+11)}\\
&+\sqrt{2(10hm+8h-6m-5)(5m+4)(n-h+1)}\Big]\\
+&\frac{2(m+1)}{5mn+2m+4n+1}\sum_{h=1}^{n}\Big[\sqrt{(10hm+8h+2m+1)((10m+8)(n-h)+2m+1)}\\
&+2\sqrt{(5mh+4h-m-1)((5m+4)(n-h)+3m+2)}\\
&+2\sqrt{(5hm+4h-2m-2)((5m+4)(n-h)+4m+3)}\Big]\\
&+\frac{2(m+1)\sqrt{(2m+1)(10mn+8n+2m+1)}}{5mn+2m+4n+1}.
\end{aligned}
$$

□

Example 1. The reader can find some values of the third geometric-arithmetic index of Titania Nanotubes $TiO_2[m,n]$ for $m,n = 10, 20, \ldots, 100, 200, \ldots 1000, 2000, \ldots, 10000, 20000, \ldots, 100000$ as follows:

$GA_3(Tio_2[10,10])$	878.299834872898
$GA_3(Tio_2[20,20])$	3326.75134599278
$GA_3(Tio_2[30,30])$	7347.23494133554
$GA_3(Tio_2[40,40])$	12938.6350668181
$GA_3(Tio_2[50,50])$	20100.9078753363
$GA_3(Tio_2[60,60])$	28834.0310643499
$GA_3(Tio_2[70,70])$	39137.9914475239
$GA_3(Tio_2[80,80])$	51012.7804601618
$GA_3(Tio_2[90,90])$	64458.3921667038
$GA_3(Tio_2[100,100])$	79474.8222529962
$GA_3(Tio_2[200,200])$	316033.662022357
$GA_3(Tio_2[300,300])$	709672.854668657
$GA_3(Tio_2[400,400])$	1260392.05217918
$GA_3(Tio_2[500,500])$	1968191.12003462
$GA_3(Tio_2[600,600])$	2833069.98931479
$GA_3(Tio_2[700,700])$	3855028.61910312
$GA_3(Tio_2[800,800])$	5034066.98275142
$GA_3(Tio_2[900,900])$	6370185.06175545
$GA_3(Tio_2[1000,1000])$	7863382.84264555
$GA_3(Tio_2[2000,2000])$	31434742.7781249
$GA_3(Tio_2[3000,3000])$	70714068.2495285
$GA_3(Tio_2[4000,4000])$	125701358.162634
$GA_3(Tio_2[5000,5000])$	196396612.093715

$GA_3(Tio_2[6000,6000])$	282799829.825484
$GA_3(Tio_2[7000,7000])$	384911011.228871
$GA_3(Tio_2[8000,8000])$	502730156.219786
$GA_3(Tio_2[9000,9000])$	636257264.739816
$GA_3(Tio_2[10000,10000])$	785492336.746446
$GA_3(Tio_2[20000,20000])$	3141781043.91026
$GA_3(Tio_2[30000,30000])$	7068866085.03745
$GA_3(Tio_2[40000,40000])$	12566747456.6702
$GA_3(Tio_2[50000,50000])$	19635425157.4688
$GA_3(Tio_2[60000,60000])$	28274899186.747
$GGA_3(Tio_2[70000,70000])$	38485169544.0965
$GA_3(Tio_2[80000,80000])$	50266236229.2508
$GA_3(Tio_2[90000,90000])$	63618099242.0258
$GA_3(Tio_2[100000,100000])$	78540758582.2871
$GA_3(Tio_2[200000,200000])$	314161149981.898
$GA_3(Tio_2[300000,300000])$	706861174083.65
$GA_3(Tio_2[400000,400000])$	1256640830876.67
$GA_3(Tio_2[500000,500000])$	1963500120356.7
$GA_3(Tio_2[600000,600000])$	2827439042521.46
$GA_3(Tio_2[700000,700000])$	3848457597369.66
$GA_3(Tio_2[800000,800000])$	5026555784900.77
$GA_3(Tio_2[900000,900000])$	6361733605114.04
$GA_3(Tio_2[1000000,1000000])$	7853991058008.67

Corollary 1. *Consider the graph of Titania Nanotubes $TiO_2[m,n]$ depicted in Fig. 2. This graph has $2(3n+2)(m+1)$ vertices and $10mn+6m+8n+4$ edges ($\forall n \in \mathbb{N}-\{1\}$). We see that*

$$
\begin{aligned}
GA_3(TiO_2[n,n]) = & \frac{2(2n+1)}{10n^2+12n+3} \\
& \times \sum_{h=1}^{n+1} \Big[\sqrt{2(5n+4)(h-1)((10n+8)(n-h)+14n+11)} \\
& + \sqrt{2(10nh+8h-6n-5)(5n+4)(n-h+1)} \Big] \\
& + \frac{2(n+1)}{5n^2+6n+1} \\
& \times \sum_{h=1}^{n} \Big[\sqrt{(10nh+8h+2n+1)((10n+8)(n-h)+2n+1)}
\end{aligned}
$$

$$+ 2\sqrt{(5nh + 4h - n - 1)((5n + 4)(n - h) + 3n + 2)}$$
$$+ 2\sqrt{(5nh + 4h - 2n - 2)((5n + 4)(n - h) + 4n + 3)}\Big]$$
$$+ \frac{(2n + 1)\sqrt{(2n + 1)(10n^2 + 10n + 1)}}{5n^2 + 6n + 1}.$$

Corollary 2. *By using Corollary 1 and the above theorem, we conclude for enough large integer number n, k:*

$$\begin{aligned} GA_3(Tio_2[10, 10]) &= 878.299834872898, \\ GA_3(Tio_2[100, 100]) &= 79475.8222529962, \\ GA_3(Tio_2[1000, 1000]) &= 7863382.84264555, \\ GA_3(Tio_2[10000, 10000]) &= 785492336.746446, \\ GA_3(Tio_2[100000, 100000]) &= 78540758582.2871, \\ GA_3(Tio_2[1000000, 1000000]) &= 7853991058008.67. \end{aligned}$$

Moreover we have following approach for the third geometric-arithmetic index of Titania Nanotubes $TiO_2[n, n]$, $\forall n = p \times 10^k$, $p, k > 1$:

$$\begin{aligned} GA_3(Tio_2[10^k, 10^k]) &\simeq 7.85 \times 10^{2k}, \\ GA_3(Tio_2[2 \times 10^k, 2 \times 10^k]) &\simeq 31.41 \times 10^{2k}, \\ GA_3(Tio_2[3 \times 10^k, 3 \times 10^k]) &\simeq 70.68 \times 10^{2k}, \\ GA_3(Tio_2[4 \times 10^k, 4 \times 10^k]) &\simeq 125.66 \times 10^{2k}, \\ GA_3(Tio_2[5 \times 10^k, 5 \times 10^k]) &\simeq 196.35 \times 10^{2k}, \\ GA_3(Tio_2[6 \times 10^k, 6 \times 10^k]) &\simeq 282.74 \times 10^{2k}, \\ GA_3(Tio_2[7 \times 10^k, 7 \times 10^k]) &\simeq 384.84 \times 10^{2k}, \\ GA_3(Tio_2[8 \times 10^k, 8 \times 10^k]) &\simeq 502.65 \times 10^{2k}, \\ GA_3(Tio_2[9 \times 10^k, 9 \times 10^k]) &\simeq 636.17 \times 10^{2k}. \end{aligned}$$

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