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On the Atom Bond Connectivity Index of Titania Nanotubes TiO_2 *(m, n)*

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Abstract

Let G(V,E) be a simple molecular graph, for a graph G(V,E) with vertex(atom) set V and the edge**(bond)** set E, the third version of atom bond connectivity index is defined as $ABC_3(G)=\sum_{e=uv\in E(G)}\sqrt{\frac{m_v+m_u-2}{m_v.m_u}}$, where m_v is the number of edges of G lying near to u than to v. In this research paper, we compute the third version of atomic-bond connectivity index of the Titania Nanotubes $TiO_2\ (m,n)$.

Keywords: Molecular graph, Titania Carbon Nanotubes $TiO_2\ (m,n)$, Orthogonal cuts, atom-bond connectivity index.

1. Introduction

Let *G(V,E)* be a simple molecular graph, where *V* and *E* are the sets of vertices(atoms) and the edges (bonds). The number of vertices in *V* is called the order and the number of edges in *E* is called the size of the graph *G*. The degree of a vertex *v*, d_v, is the number of adjacent vertices with *v*. The length of the shortest path between two vertices *u* and *v* is called the distance and is denoted by $d(u,v)$.

A topological index is a real number associated with a molecular graph, this real number predict the certain physical or chemical properties of that molecule. A lot of degree, distance and spectrum based topological indices have been introduced. For more details see [1-6].

The very first degree based topological index is Randic Index [7] introduced by *Milan Randic* as

$$\chi(G)=\sum_{\{u,v\}\in E(G)}\frac{1}{\sqrt{d_u d_v}}$$

Estrada et al. [8] proposed the atom-bond connectivity (ABC) index. It is defined as

$$ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_u d_v}}.$$

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Estrada *et al*. developed a basically topological approach on the basis of the ABC index which explains the differences in the energy of linear and branched alkanes both qualitatively and quantitatively. Furtula et al. [2] determined the extremal (minimum and maximum) values of this index for chemical trees and showed that the star is the unique tree with the maximum ABC index. This index has proven to be a valuable predictive index in the study of the formation heat in alkanes [8].
One can consult [3, 4, 6, 9, 10] for recent results on vertex-degree based topological indices.
I. Gutman [11] introduced the distance based topological index named *Szeged index*. Then for an edge $e=uv\in E(G)$, suppose that
$m_u(e|G)=\{x|x\in E(G),d(u,x)<d(x,v)\}$,
$m_v(e|G)=\{x|x\in E(G),d(v,x)<d(x,u)\}$,

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

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

I. Gutman et al. [12] proposed the edge version of Szeged index. This version of Szeged index is defined as

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

Readers are encouraged to see [1-7, 12, 13] for computations of this index for some graph.
The *third atom-bond connectivity index* of a graph G is defined as

$$ABC_3(G)=\sum_{e=uv\in E(G)}\sqrt{\frac{m_v+m_u-2}{m_v.m_u}}.$$

Titania nanotube (TiO_2) is among the most studied compounds in materials science. This material has application in various fields for examples biomedical sciences like used in photo catalysis, dye-sensitized solar cells etc. In this research paper, we computed the third version of ABC index of titania nanotube.

2. Main Results and Discussions

Let G be the graph of $TiO_2(m,n)$ for all $m,n\in N$ depicted in Figure-1 This graph has $2(3n+2)(m+1)$ vertices/ atoms and $10mn+6m+8n+4$ edges (bonds). By using the edge partition, the graph has $2mn+4n+4$ atoms of degree two, $2n$ atoms of degree four, $2mn$ atoms with degree five and the atoms of degree three are $2mn+4m$. For more information and details see [14-27].
Our aim to compute the atom bond connectivity index of G 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 $m_v(e|TiO_2(m,n)$ based on orthogonal cuts of G with $5n+3$ vertical cuts for horizontal edges. Let e being an oblique edge we denote its orthogonal cut by C_i *or* F_j $\forall i=1,2,.....2(n+1)$ *and* $j=1,....3n+1$.
Note that the sizes of all orthogonal cuts are equivalent with $|C_i|=2m+1$ and $|F_i|=2(m+1)$.

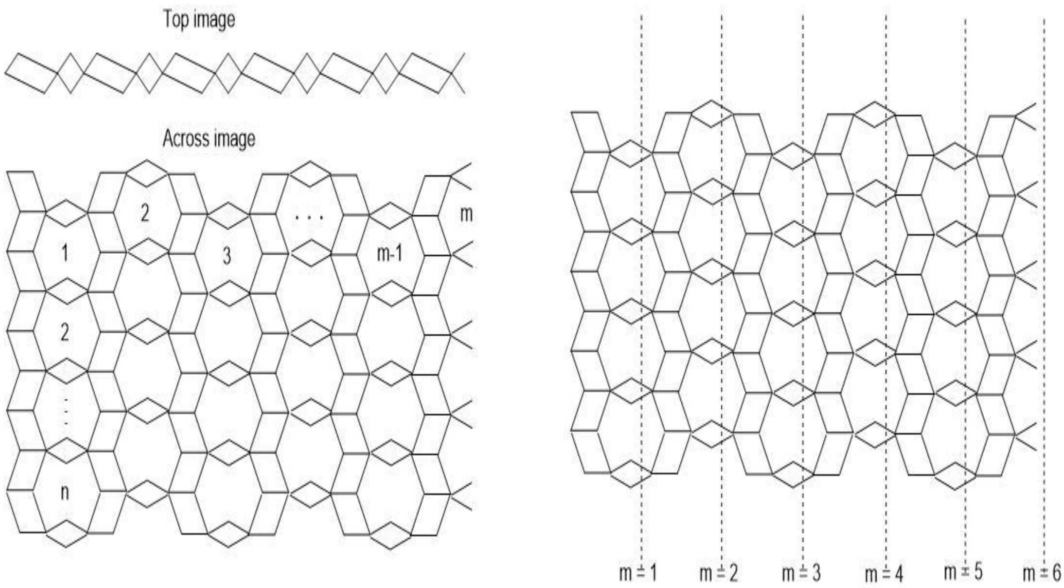

Figure 1- Titania Nanotubes $TiO_2\,[m,n]$ [14, 15].

In case the orthogonal cuts $C_i\ (i=1,\ldots,2(n+1)$, see Figure-2: The values C_i are classified as following:

1. For C_1:

$m_u(e_1|TiO_2(m,n)=0$and$m_v(e_1|TiO_2(m,n)=|E(TiO_2(m,n)|-|C_1|=10mn+6m+8n+4-(2m+1)=10mn+4m+8n+3$.

2. For C_2:

$m_u(e_2|TiO_2(m,n)=|C_1|+|F_1|=2m+1+2m+2=4m+3$ and
$m_v(e_2|TiO_2(m,n)=|E(TiO_2(m,n)|-(|C_1|+|F_1|+|C_2|)=10mn+6m+8n+4-(6m+4)=10mn+2m+8n.$

3. For C_3:

$m_u(e_3|TiO_2(m,n)=2|C_1|+3|F_1|=10m+8andm_v(e_3|TiO_2(m,n)=|E(TiO_2(m,n)|-(3|C_1|+3|F_1|)=10mn+6m+8n+4-(12m+9)=10mn+8n-6m-5.$

4. For C_4:

$m_u(e_4|TiO_2(m,n)=3|C_1|+4|F_1|=14m+11andm_v(e_4|TiO_2(m,n)=|E(TiO_2(m,n)|-(3|C_1|+4|F_1|)=10mn+6m+8n+4-(16m+12)=10mn+8n-10m-8$

5. 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
$m_v(e_{(2h-1)}|TiO_2(m,n)=|E(TiO_2(m,n)|-((2h-1)|C_1|+(3h-3)|F_1|)$
$=10mn+6m+8n+4-(10m+8)(h-1)\,-(2m+1)$

6. 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
$m_v(e_{(2h)}|TiO_2(m,n)=|E(TiO_2(m,n)|-(2h|C_1|+(3h-1)|F_1|)=10m(n-h)+10m+8(n-h)+8.$

7. 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 case the orthogonal cuts $F_j\ (j=1,\ldots,3n+1)$, *see* Figure-2*:*

1. **ForF_1:** $m_u(e_1|TiO_2(m,n)=2m+1=|C_i|$ *and*
$m_v(e_1|TiO_2(m,n)=|E(TiO_2(m,n)|-(|C_1|+|F_1|)=10mn+6m+8n+4-(4m+3)=10mn+8n+2m+1.$
2. **ForF_2:** $m_u(e_2|TiO_2(m,n)=2|C_1|+|F_1|=6m+4$ *and*
$m_v(e_2|TiO_2(m,n)=|E(TiO_2(m,n)|-(2|C_1|+2|F_1|)=10mn+6m+8n+4-(8m+6)=10mn+8n-2m-2.$
3. **ForF_3:** $m_u(e_3|TiO_2(m,n)=2|C_1|+2|F_1|=8m+6$ *and*
$m_v(e_3|TiO_2(m,n)=|E(TiO_2(m,n)|-(2|C_1|+3|F_1|)=10mn+6m+8n+4-(10m+8)=10mn+8n-4m-4.$
4. **ForF_4:** $m_u(e_4|TiO_2(m,n)=3|C_1|+3|F_1|=12m+9$ *and*
$m_v(e_4|TiO_2(m,n)=|E(TiO_2(m,n)|-(3|C_1|+4|F_1|)=10mn+6m+8n+4-(14m+11)=10mn+8n-8m-7.$
5. **For F_5:** $m_u(e_5|TiO_2(m,n)=4|C_1|+4|F_1|=16m+12$ *and*
$m_v(e_5|TiO_2(m,n)=|E(TiO_2(m,n)|-(4|C_1|+5|F_1|)=10mn+6m+8n+4-(18m+14)=10mn+8n-12m-10.$

6. For F_6: $m_u(e_6|TiO_2(m,n)=4|C_1|+5|F_1|=18m+13$ and
$m_v(e_6|TiO_2(m,n)=|E(TiO_2(m,n)|-(4|C_1|+6|F_1|)=10mn+6m+8n+4-(20m+15)=10mn+8n-14m-11$.

7. For F_7: $m_u(e_7|TiO_2(m,n)=5|C_1|+6|F_1|=22m+17$ and
$m_v(e_7|TiO_2(m,n)=|E(TiO_2(m,n)|-(4|C_1|+6|F_1|)=10mn+6m+8n+4-(24m+19)$.

8. For F_8: $m_u(e_8|TiO_2(m,n)=6|C_1|+7|F_1|=22m+17$ and
$m_v(e_8|TiO_2(m,n)=|E(TiO_2(m,n)|-(4|C_1|+6|F_1|)=10mn+6m+8n+4-(24m+19)$.

9. For F_{3h+1} $(h=0,\ldots,n)$:
$m_u(F_{3h+1}|TiO_2(m,n)=(2h+1)|C_1|+(3h)|F_1|=(2h+1)(2m+1)+(3h)\,(2m+2)=10hm+2m+8h+1$.
$m_v(F_{3h+1}|TiO_2(m,n)=|E(TiO_2(m,n)|-(10hm+4m+8h+3)=(10m+8)(n-h)+2m+1$.

10. For F_{3h-1} $(h=1,\ldots,n)$:
$m_u\,(F_{3h-1}|TiO_2(m,n)=(2h)|C_1|+(3h-2)|F_1|=(2h)(2m+1)+(3h-2)$
$(2m+2)=(10m+8)h-2|F_1|=10hm-4m+8h-4$.
$m_v(F_{3h-1}|TiO_2(m,n)=(10mn+6m+8n+4)-(10hm-2m+8h-2)=(10m+8)(n-h)+8m+6$.

11. For F_{3h} $(h=1,\ldots,n)$:
$m_u\,(F_{3h}|TiO_2(m,n)=m_u(F_{3h-1}|TiO_2(m,n)+|F_1|$
$k2=2h|C_1|+(3h-1)|F_1|=(10m+8)h-|F_1|=(10m+8)h-2m-2$.
$m_v(F_{3h}|TiO_2(m,n)=m_v(F_{3h-1}|TiO_2(m,n)-|F_1|=(10m+8)(n-h)+6m+4$.

Based on the above calculations we have two following results.

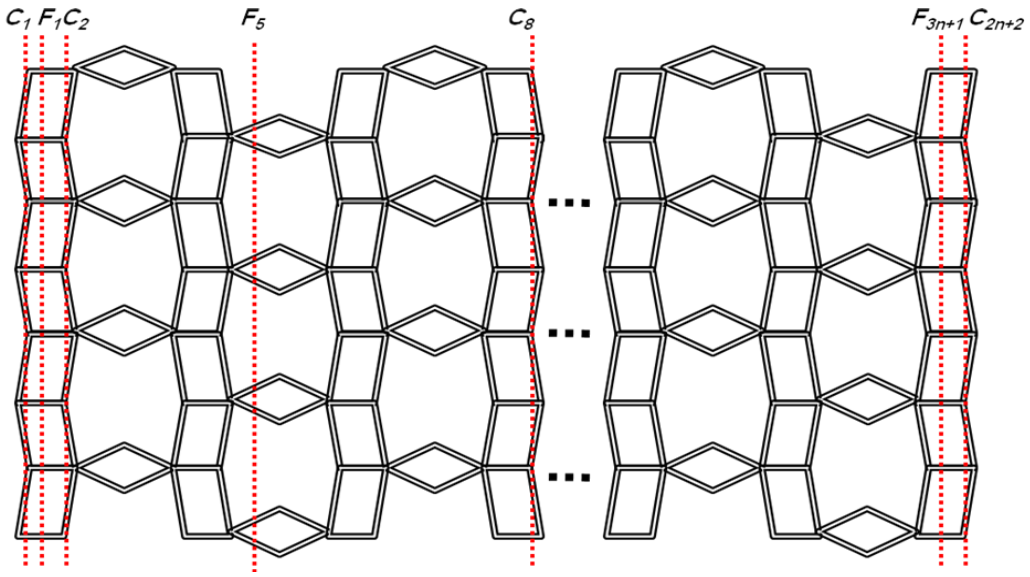

Figure 2- [16-19] Orthogonal cuts representation of the Titania Nanotubes.

Theorem 2-1 The third atom-bond connectivity index (ABC_3) of Titania Nanotubes $(TiO_2\,[m,n])$ is equal to

$$ABC_3\left(TiO_2\left[m,n\right]\right)=(2m+1)\sqrt{10mn+4m+8n+1}\sum_{h=2}^{n+1}\left[\left(2\left(5m+4\right)\left(h-1\right)\left(\left(10m+8\right)\left(n-h\right)+14m+11\right)\right)^{-0.5}\right]$$

$$+(2m+1)\sqrt{10mn+4m+8n+1}\sum_{h=1}^{n}\left[\left(2\left(10hm+8h-6m-5\right)\left(5m+4\right)\left(n-h+1\right)\right)^{-0.5}\right]$$

$$+\,(2m+2)\sqrt{10mn+4m+8n}\sum_{h=0}^{n}\left[\begin{array}{l}\left(10hm+8h+2m+1\right)^{-0.5}\left(\left(10m+8\right)\left(n-h\right)+2m+1\right)^{-0.5}\\+\frac{1}{2}\left(5mh+4h-m-1\right)^{-0.5}\left(\left(5m+4\right)\left(n-h\right)+3m+2\right)^{-0.5}\\+\frac{1}{2}\left(5hm+4h-2m-2\right)^{-0.5}\left(\left(5m+4\right)\left(n-h\right)+4m+3\right)^{-0.5}\end{array}\right]$$

Proof:

From the definition of third atom bond connectivity index and the calculation done early in this section we have

$$ABC_3(TiO_2(m,n)) = \sum_{e_i=uv\in E(TiO_2(m,n))} \sqrt{\frac{m_v + m_u - 2}{m_v . m_u}}$$

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

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

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

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

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

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

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

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

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

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

$$+ 2(m+1) \sum_{\substack{f_{3h}=vu\in F_{3k} \\ h=0,\dots,n}} \left[\sqrt{\frac{((10m+8)h - 2m - 2) + \left((10m+8)(n-h) + 6m+4\right) - 2}{((10m+8)h - 2m - 2) \times \left((10m+8)(n-h) + 6m+4\right)}} \right]$$

$$+ 2(m+1) \sum_{\substack{f_{3h-1}=vu\in F_{3k-1} \\ h=0,\dots,n}} \left[\sqrt{\frac{(10hm-4m+8h-4) \times \left((10m+8)(n-h) + 8m+6\right) - 2}{(10hm-4m+8h-4) \times \left((10m+8)(n-h) + 8m+6\right)}} \right]$$

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

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

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

$$+2(m+1)\sum_{\substack{f_{3h}=vu\in F_{3k}\\ h=0,\ldots,n}}\left[\sqrt{\frac{10mn+4m+8n}{(10mh+8h-2m-2)(10mn-10mh+8n-8h+6m+4)}}\right]$$

$$+2(m+1)\sum_{\substack{f_{3h-1}=vu\in F_{3k-1}\\ h=0,\ldots,n}}\left[\sqrt{\frac{10mn+4m+8n}{(10hm-4m+8h-4)\times(10mn-10mh+8n-8h+8m+6)}}\right]$$

$$=(2m+1)\sqrt{10mn+4m+8n+1}\sum_{h=1}^{n+1}\left[\begin{array}{l}(10mh+8h-10m-8)^{-0.5}(10mn-10mh-8h+14m+8n+11)^{-0.5}\\+(10hm+8h-6m-5)^{-0.5}(10mn-10mh-8h+10m+8n+8)^{-0.5}\end{array}\right]$$

$$+\ (2m+2)\sqrt{10mn+4m+8n}\sum_{h=0}^{n}\left[\begin{array}{l}(10hm+2m+8h+1)^{-0.5}(10mn-10mh+8n-8h+2m+1)^{-0.5}\\+(10mh+8h-2m-2)^{-0.5}(10mn-10mh+8n-8h+6m+4)^{-0.5}\\+(10hm-4m+8h-4)^{-0.5}(10mn-10mh+8n-8h+8m+6)^{-0.5}\end{array}\right]$$

$$=(2m+1)\sqrt{10mn+4m+8n+1}\sum_{h=1}^{n+1}\left[\begin{array}{l}\left(2(5m+4)(h-1)\left((10m+8)(n-h)+14m+11\right)\right)^{-0.5}\\+\left(2(10hm+8h-6m-5)(5m+4)(n-h+1)\right)^{-0.5}\end{array}\right]$$

$$+\ (2m+2)\sqrt{10mn+4m+8n}\sum_{h=0}^{n}\left[\begin{array}{l}(10hm+8h+2m+1)^{-0.5}\left((10m+8)(n-h)+2m+1\right)^{-0.5}\\+\frac{1}{2}(5mh+4h-m-1)^{-0.5}\left((5m+4)(n-h)+3m+2\right)^{-0.5}\\+\frac{1}{2}(5hm+4h-2m-2)^{-0.5}\left((5m+4)(n-h)+4m+3\right)^{-0.5}\end{array}\right]$$

$$=(2m+1)\sqrt{10mn+4m+8n+1}\sum_{h=2}^{n+1}\left[\left(2(5m+4)(h-1)\left((10m+8)(n-h)+14m+11\right)\right)^{-0.5}\right]$$

$$+(2m+1)\sqrt{10mn+4m+8n+1}\sum_{h=1}^{n}\left[\left(2(10hm+8h-6m-5)(5m+4)(n-h+1)\right)^{-0.5}\right]$$

$$+\ (2m+2)\sqrt{10mn+4m+8n}\sum_{h=0}^{n}\left[\begin{array}{l}(10hm+8h+2m+1)^{-0.5}\left((10m+8)(n-h)+2m+1\right)^{-0.5}\\+\frac{1}{2}(5mh+4h-m-1)^{-0.5}\left((5m+4)(n-h)+3m+2\right)^{-0.5}\\+\frac{1}{2}(5hm+4h-2m-2)^{-0.5}\left((5m+4)(n-h)+4m+3\right)^{-0.5}\end{array}\right].+$$

Corollary 2-1 Consider the graph of Titania Nanotubes *($TiO_2[m,n]$)* depicted in Figure-2, thus
$ABC_3(TiO_2(n,n))$

$$=(2n+1)\sqrt{10n^2+12n+1}\sum_{h=2}^{n+1}\left[\left(2(5n+4)(h-1)\left((10n+8)(n-h)+14n+11\right)\right)^{-0.5}\right]$$

$$+(2n+1)\sqrt{10n^2+12n+1}\sum_{h=1}^{n}\left[\left(2(10hn+8h-6m-5)(5n+4)(n-h+1)\right)^{-0.5}\right]$$

$$+\ 2(n+1)\sqrt{10n^2+12n}\sum_{h=0}^{n}\left[\begin{array}{l}(10nh+8h+2n+1)^{-0.5}\left((10n+8)(n-h)+2n+1\right)^{-0.5}\\+\frac{1}{2}(5nh+4h-n-1)^{-0.5}\left((5n+4)(n-h)+3n+2\right)^{-0.5}\\+\frac{1}{2}(5nh+4h-2n-2)^{-0.5}\left((5n+4)(n-h)+4n+3\right)^{-0.5}\end{array}\right]$$

Example 2-1 By $ABC_3(TiO_2(n,n))$ from Theorem 2-1 and Corollary 2-1 we can compute some values of the third atom-bond connectivity index *(ABC_3)* of Titania Nanotubes $TiO_2[n,n]$ in cases *n=10,20,…, 100,200,… 1000, 2000,…, 10000,20000,…, 100000* as follows:

ABC3(Tio2[10,10])	189.471697164843	ABC3(Tio2[6000,6000])	130133.909653037
ABC3(Tio2[20,20])	391.487186003641	ABC3(Tio2[7000,7000])	151908.517175455
ABC3(Tio2[30,30])	597.131141691419	ABC3(Tio2[8000,8000])	173688.764745554
ABC3(Tio2[40,40])	804.729712667658	ABC3(Tio2[9000,9000])	195473.621746691
ABC3(Tio2[50,50])	1013.59838300573	ABC3(Tio2[10000,10000])	217262.33776623
ABC3(Tio2[60,60])	1223.37763792512	ABC3(Tio2[20000,20000])	435279.414451257
ABC3(Tio2[70,70])	1433.85097603564	ABC3(Tio2[30000,30000])	653423.028535021
ABC3(Tio2[80,80])	1644.87607484862	ABC3(Tio2[40000,40000])	871632.145006282
ABC3(Tio2[90,90])	1856.3534555217	ABC3(Tio2[50000,50000])	1089883.12161511
ABC3(Tio2[100,100])	2068.21035019857	ABC3(Tio2[60000,60000])	1308163.83297695
ABC3(Tio2[200,200])	4199.61273279957	ABC3(Tio2[70000,70000])	1526467.07598731
ABC3(Tio2[300,300])	6343.56697894067	ABC3(Tio2[80000,80000])	1744788.15739478
ABC3(Tio2[400,400])	8494.03953630257	ABC3(Tio2[90000,90000])	1963123.8172407
ABC3(Tio2[500,500])	10648.6833454523	ABC3(Tio2[100000,100000])	2181471.68196077
ABC3(Tio2[600,600])	12806.2923999935	ABC3(Tio2[200000,200000])	4365361.20101551
ABC3(Tio2[700,700])	14966.1494849107	ABC3(Tio2[300000,300000])	6549650.89257744
ABC3(Tio2[800,800])	17127.7869546141	ABC3(Tio2[400000,400000])	8734147.72923624
ABC3(Tio2[900,900])	19290.8798131657	ABC3(Tio2[500000,500000])	10918776.943184
ABC3(Tio2[1000,1000])	21455.191341262	ABC3(Tio2[600000,600000])	13103500.1888751
ABC3(Tio2[2000,2000])	43139.3483679292	ABC3(Tio2[700000,700000])	15288294.6872743
ABC3(Tio2[3000,3000])	64863.4930266201	ABC3(Tio2[800000,800000])	17473145.596571
ABC3(Tio2[4000,4000])	86608.3427742496	ABC3(Tio2[900000,900000])	19658042.607603
ABC3(Tio2[5000,5000])	108366.42585807	ABC3(Tio2[1000000,1000000])	21842978.2143297

Corollary 2-2. By using the above table and Corollary 2-1 we have following approach for ABC_3 of Titania Nanotubes $TiO_2[n,n]$ for enough large integer number $m,n,k,p\geq 1$, where in $TiO_2[m,n]$, $m = n = p\times 10^k$:

$$ABC_3\left(TiO_2\left[10^k, 10^k\right]\right) = 2.185\times 10^{k+1}$$

$$ABC_3\left(TiO_2\left[2\times10^k, 2\times10^k\right]\right) = 4.365\times10^{k+1}$$
$$ABC_3\left(TiO_2\left[3\times10^k, 3\times10^k\right]\right) = 6.5 \times10^{k+1}$$
$$ABC_3\left(TiO_2\left[4\times10^k, 4\times10^k\right]\right) = 8.734\times10^{k+1}$$
$$ABC_3\left(TiO_2\left[5\times10^k, 5\times10^k\right]\right) = 1.092\times10^{k+2}$$
$$ABC_3\left(TiO_2\left[6\times10^k, 6\times10^k\right]\right) = 1.31\times10^{k+2}$$
$$ABC_3\left(TiO_2\left[7\times10^k, 7\times10^k\right]\right) = 1.53\times10^{k+2}$$
$$ABC_3\left(TiO_2\left[8\times10^k, 8\times10^k\right]\right) = 1.75\times10^{k+2}$$
$$ABC_3\left(TiO_2\left[9\times10^k, 9\times10^k\right]\right) = 1.97\times10^{k+2}.$$

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