On the Atom Bond Connectivity Index of Titania Nanotubes $\text{TiO}_2(m, n)$

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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 $ABC_3(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{m_u + m_v - 2}{m_u m_v}}$, 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 $\text{TiO}_2(m, n)$.

Keywords: Molecular graph, Titania Carbon Nanotubes $\text{TiO}_2(m,n)$, 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

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

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

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

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

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

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

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 $2(3n+2)(m+1)$ vertex/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 $|F_j| = 2(m+1)$.
In case the orthogonal cuts $F_i (i=1,...,2(n+1))$, see Figure-2: The values $C_i$ are classified as following:

1. For $C_1$:
   
   $m_i(e_1)\text{[TiO}_2(m,n)]=0\text{and }m_i(e_1)\text{[TiO}_2(m,n)]=|E(\text{TiO}_2(m,n)|-|C_i|=10mn+6m+8n+4(2m+1)=10mn+4m+8n+3$.

2. For $C_2$:
   
   $m_i(e_2)\text{[TiO}_2(m,n)]=|C_i|+|F_i|=2m+1+2m+2=4m+3$ and
   $m_i(e_2)\text{[TiO}_2(m,n)]=|E(\text{TiO}_2(m,n)|-|C_i|+|F_i|=10mn+6m+8n+4(6m+4)=10mn+2m+8n$.

3. For $C_3$:
   
   $m_i(e_3)\text{[TiO}_2(m,n)]=2|C_i|+3|F_i|=10m+8|\text{and }m_i(e_3)\text{[TiO}_2(m,n)]=|E(\text{TiO}_2(m,n)|-3|C_i|+3|F_i|=10mn+6m+8n+4(12m+9)=10mn+8n+6n-6m-5$.

4. For $C_4$:
   
   $m_i(e_4)\text{[TiO}_2(m,n)]=3|C_i|+4|F_i|=14m+11\text{and }m_i(e_4)\text{[TiO}_2(m,n)]=|E(\text{TiO}_2(m,n)|-3|C_i|+4|F_i|=10mn+6m+8n+4(16m+12)=10mn+8n-10m-8$.

5. For $C_{2n+1}$:
   
   $m_i(e_{2n+1})\text{[TiO}_2(m,n)]=(2h-2)|C_i|+(3h-3)|F_i|=(2h-2)(2m+1)+(3h-3)(2m+2)=(10m+8)(h-1)$ and
   $m_i(e_{2n+1})\text{[TiO}_2(m,n)]=|E(\text{TiO}_2(m,n)|-(2h)|C_i|+(3h-3)|F_i|)=10mn+6m+8n+4(10m+8)(h-1)-(2m+1)$.

6. For $C_{2n+2}$:
   
   $m_i(e_{2n+2})\text{[TiO}_2(m,n)]=(2h+1)|C_i|+(3h+1)|F_i|=(2h+1)(2m+1)+(3h+2)(2m+2)=10hm+8h-6m-5$ and
   $m_i(e_{2n+2})\text{[TiO}_2(m,n)]=|E(\text{TiO}_2(m,n)|-(2h+1)|C_i|+(3h+1)|F_i|)=10m(n-h)+10m+8n(8n-h)+8$.

7. For $C_{2n+3}$:
   
   $m_i(e_{2n+3})\text{[TiO}_2(m,n)]=(2n+1)|C_i|+(3n+1)|F_i|=(2n+1)(2m+1)+(3n+2)(2m+2)=10mn+8n+4m+3$ and
   $m_i(e_{2n+3})\text{[TiO}_2(m,n)]=0$.

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

1. For $F_1$:
   
   $m_j(e_1)\text{[TiO}_2(m,n)=2m+1|=|C_i|$ and
   $m_j(e_1)\text{[TiO}_2(m,n)=|E(\text{TiO}_2(m,n)|-|C_i|+|F_j|=10mn+6m+8n+4(4m+3)=10mn+8n+2m+1$.

2. For $F_2$:
   
   $m_j(e_2)\text{[TiO}_2(m,n)=2|C_i|+|F_j|=6m+4$ and
   $m_j(e_2)\text{[TiO}_2(m,n)=|E(\text{TiO}_2(m,n)|-2|C_i|+2|F_j|=10mn+6m+8n+4(8m+6)=10mn+8n-2m+2$.

3. For $F_3$:
   
   $m_j(e_3)\text{[TiO}_2(m,n)=3|C_i|+3|F_j|=8m+6$ and
   $m_j(e_3)\text{[TiO}_2(m,n)=|E(\text{TiO}_2(m,n)|-3|C_i|+3|F_j|=12m+9$ and
   $m_j(e_3)\text{[TiO}_2(m,n)=|E(\text{TiO}_2(m,n)|-3|C_i|+4|F_j|=10mn+6m+8n+4(14m+11)=10mn+8n-8m-7$.

4. For $F_4$:
   
   $m_j(e_4)\text{[TiO}_2(m,n)=4|C_i|+4|F_j|=16m+12$ and
   $m_j(e_4)\text{[TiO}_2(m,n)=|E(\text{TiO}_2(m,n)|-4|C_i|+5|F_j|=10mn+6m+8n+4(18m+14)=10mn+8n-12m-10$.
6. **For F₈**: \( m_\delta(e₄[TiO₂(m,n)]=4|C₁|+5|F₁|=18m+13 \) and
\( m_\delta(e₄[TiO₂(m,n)]=|E[TiO₂(m,n)]-(4|C₁|+6|F₁|)=10mn+6m+8n+4-(20m+15)=10mn+8n-14m-11. \)

7. **For F₇**: \( m_\delta(e₄[TiO₂(m,n)]=5|C₁|+6|F₁|=22m+17 \) and
\( m_\delta(e₄[TiO₂(m,n)]=|E[TiO₂(m,n)]-(5|C₁|+6|F₁|)=10mn+6m+8n+4-(24m+19). \)

8. **For F₆**: \( m_\delta(e₄[TiO₂(m,n)]=6|C₁|+7|F₁|=22m+17 \) and
\( m_\delta(e₄[TiO₂(m,n)]=|E[TiO₂(m,n)]-(6|C₁|+7|F₁|)=10mn+6m+8n+4-(24m+19). \)

9. **For F₃ₕₜ (h=0, ..., n)**:
\( m_\delta(F₃ₕₜ[TiO₂(m,n)]=2(h+1)|C₁|+(3h)|F₁|=(2h+1)(2m+1)+(3h)(2m+2)=10hm+2m+8h+1. \)
\( m_\delta(F₃ₕₜ[TiO₂(m,n)]=|E[TiO₂(m,n)]-(10hm+4m+8h+3)=(10m+8)(n-h)+2m+1. \)

10. **For F₃ₜ (h=1, ..., n)**:
\( m_\delta(F₃ₜ[TiO₂(m,n)]=10m+6m+8n+4)-(10hm-2m+8h-2)=(10m+8)(n-h)+8m+6. \)

11. **For F₃ₜ (h=1, ..., n)**:
\( m_\delta(F₃ₜ[TiO₂(m,n)]=|m_\delta(F₃ₜ[TiO₂(m,n)]+|F₁|)
\( k₂=2h|C₁|+(3h-1)|F₁|=(10m+8)h|F₁|=(10m+8)h-2m-2. \)
\( m_\delta(F₃ₜ[TiO₂(m,n)]=m_\delta(F₃ₜ[TiO₂(m,n)]-|F₁|=(10m+8)(n-h)+6m+4. \)

Based on the above calculations we have two following results.

![Orthogonal cuts representation of the Titania Nanotubes](image)

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

**Theorem 2-1** The third atom-bond connectivity index \((ABC₃)\) of Titania Nanotubes \((TiO₂[m,n])\) is equal to
\[
ABC₃(TiO₂[m,n]) = (2m+1)\sqrt[0.5]{10mn+4m+8n+4}\sum_{h=0}^{n} \left[ (2(5m+4)(h-1)(10m+8)(n-h)+14m+11) \right]^{0.5} + (2m+1)\sqrt[0.5]{10mn+4m+8n+4}\sum_{h=0}^{n} \left[ (10hm+8h+2m+1) \right]^{0.5} + (2m+2)\sqrt[0.5]{10mn+4m+8n+4}\sum_{h=0}^{n} \left[ (5mh+4h-2m-2) \right]^{0.5}
\]

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Proof:

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

\[
ABC_3(TiO_2(m,n)) = \sum_{e_{vu} \in E(TiO_2(m,n))} \sqrt{m_v + m_u - 2}
\]

\[
= \sum_{e_{vu} \in E(TiO_2(m,n))} |C| \left[ \sqrt{m_v (e_{vu} |TiO_2(m,n)|) + m_u (e_{vu} |TiO_2(m,n)|) - 2} \right]
\]

\[
= \sum_{e_{vu} \in E(TiO_2(m,n))} |F| \left[ \sqrt{m_v (f_{vu} |TiO_2(m,n)|) + m_u (f_{vu} |TiO_2(m,n)|) - 2} \right]
\]

\[
= (2m + 1) \sum_{e_{vu} \in E(TiO_2(m,n))} \left[ \sqrt{(10m + 8)(h - 1) + (10mn + 8n + 6m + 4) - (10m + 8)(h - 1) - (2m + 1)} \right]
\]

\[
+ (2m + 1) \sum_{e_{vu} \in E(TiO_2(m,n))} \left[ \sqrt{(10m + 8)h - 6m - 5) + (10m(n - h) + 10m + 8(n - h) + 8) - 2} \right]
\]

\[
+ 2(m + 1) \sum_{e_{vu} \in E(TiO_2(m,n))} \left[ \sqrt{(10hm + 2m + 8h + 1) + \left( (10m + 8)(n - h) + 2m + 1 \right) - 2} \right]
\]

\[
+ 2(m + 1) \sum_{e_{vu} \in E(TiO_2(m,n))} \left[ \sqrt{(10m + 8)h - 2m - 2) + \left( (10m + 8)(n - h) + 6m + 4) - 2} \right]
\]

\[
+ 2(m + 1) \sum_{e_{vu} \in E(TiO_2(m,n))} \left[ \sqrt{(10hm - 4m + 8h - 4) + \left( (10m + 8)(n - h) + 8m + 6) - 2} \right]
\]

\[
= (2m + 1) \sum_{e_{vu} \in E(TiO_2(m,n))} \left[ \sqrt{10mn + 4m + 8n + 1} \right]
\]

\[
+ (2m + 1) \sum_{e_{vu} \in E(TiO_2(m,n))} \left[ \sqrt{10hm + 8h - 6m - 5) + (10mn - 10mh - 8h + 14m + 8n + 11) \right]
\]

\[
= (2m + 1) \sum_{e_{vu} \in E(TiO_2(m,n))} \left[ \sqrt{10mn + 4m + 8n + 1} \right]
\]

\[
+ (2m + 1) \sum_{e_{vu} \in E(TiO_2(m,n))} \left[ \sqrt{10hm + 8h - 6m - 5) + (10mn - 10mh - 8h + 14m + 8n + 11) \right]
\]

\[
= (2m + 1) \sum_{e_{vu} \in E(TiO_2(m,n))} \left[ \sqrt{10mn + 4m + 8n + 1} \right]
\]
\[+2(m+1) \sum_{i=0,...,n} \sqrt{\frac{10mn+4m+8n}{(10hm+2m+8h+1)\times(10mn-10mh+8n-8h+2m+1)}}\]

\[+2(m+1) \sum_{i=0,...,n} \sqrt{\frac{10mn+4m+8n}{(10mh+8h-2m-2)(10mn-10mh+8n-8h+6m+4)}}\]

\[+2(m+1) \sum_{i=0,...,n} \sqrt{\frac{10mn+4m+8n}{(10hm-4m+8h-4)(10mn-10mh+8n-8h+8m+6)}}\]

\[=(2m+1)\sqrt{10mn+4m+8n+1} \sum_{h=0}^{n+1} \left[ (10hm+8h-10m-8)^{0.5} (10mn-10mh-8h+14m+8n+11)^{0.5} \right] \]

\[+(2m+2)\sqrt{10mn+4m+8n+1} \sum_{h=0}^{n+1} \left[ (10hm+8h+2m+1)^{0.5} (10mn-10mh+8h-10m+8n+11)^{0.5} \right] \]

\[+(2m+2)\sqrt{10mn+4m+8n+1} \sum_{h=0}^{n+1} \left[ (10hm+8h+2m+1)^{0.5} (10mn-10mh+8h-10m+8n+11)^{0.5} \right] \]

\[+(2m+2)\sqrt{10mn+4m+8n+1} \sum_{h=0}^{n+1} \left[ (10hm+8h+2m+1)^{0.5} (10mn-10mh+8h-10m+8n+11)^{0.5} \right] \]

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

\[=(2n+1)\sqrt{10n^2+12n+1} \sum_{h=0}^{n+1} \left[ (2(5m+4)(h-1)((10n+8)(n-h)+14m+11))^{0.5} \right] \]

\[+(2n+1)\sqrt{10n^2+12n+1} \sum_{h=0}^{n+1} \left[ (2(10hn+8h-6m-5)(5m+4)(n-h+1))^{0.5} \right] \]

\[+(2n+1)\sqrt{10n^2+12n+1} \sum_{h=0}^{n+1} \left[ (10hn+8h+2n+1)^{0.5} (10n+8)(n-h+2n+1)^{0.5} \right] \]

\[+2(n+1)\sqrt{10n^2+12n+1} \sum_{h=0}^{n+1} \left[ (10hn+8h+2n+1)^{0.5} (10n+8)(n-h+2n+1)^{0.5} \right] \]

**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 \(n=10,20,\ldots, 100,200,\ldots, 1000, 2000,\ldots, 10000,20000,\ldots, 100000\) as follows:
Corollary 2-2. By using the above table and Corollary 2-1 we have following approach for ABC3 of Titania Nanotubes TiO2[n,n] for enough large integer number m,n,k,p≥1, where in TiO2[m,n], m = n = p × 10^k:

\[
ABC_3(TiO_2[^{10^k},10^k]) = 2.185 \times 10^{k+1}
\]
\[ ABC_3(TiO_2\left[2\times10^4,2\times10^4\right]) = 4.365 \times 10^{4.1} \]
\[ ABC_3(TiO_2\left[3\times10^4,3\times10^4\right]) = 6.5 \times 10^{4.1} \]
\[ ABC_3(TiO_2\left[4\times10^4,4\times10^4\right]) = 8.734 \times 10^{4.1} \]
\[ ABC_3(TiO_2\left[5\times10^4,5\times10^4\right]) = 1.092 \times 10^{4.2} \]
\[ ABC_3(TiO_2\left[6\times10^4,6\times10^4\right]) = 1.31 \times 10^{4.2} \]
\[ ABC_3(TiO_2\left[7\times10^4,7\times10^4\right]) = 1.53 \times 10^{4.2} \]
\[ ABC_3(TiO_2\left[8\times10^4,8\times10^4\right]) = 1.75 \times 10^{4.2} \]
\[ ABC_3(TiO_2\left[9\times10^4,9\times10^4\right]) = 1.97 \times 10^{4.2} \]

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