ON SOME DEGREE BASED TOPOLOGICAL INDICES OF TiO_2 NANOTUBES

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Two well known connectivity topological indices are the atom-bond connectivity index and the geometric-arithmetic index, introduced by Estrada et al. and Vukičević et al. respectively. In this paper, we calculate the first and fourth version of ABC index and the first and fifth version of GA index of an infinite class of titania nanotubes $TiO_2[m, n]$

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1. Introduction

Mathematical chemistry is a branch of theoretical chemistry in which we discuss and predict the chemical structure by using mathematical tools. Chemical graph theory is a branch of mathematical chemistry in which we apply tools from graph theory to model the chemical phenomenon mathematically. This theory plays a prominent role in the fields of chemical sciences.

A molecular graph is a simple graph in which vertices denote the atoms and edges denote the chemical bonds in underlying chemical structure. The hydrogen atoms are often omitted in a molecular graph. Let G be a molecular graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. The order and size of G are defined as $|V(G)|$ and $|E(G)|$, respectively. An edge in $E(G)$ with end vertices u and v is denoted by uv.

A topological index is a molecular graph invariant which correlates the physico-chemical properties of a molecular graph with a number [13]. The first topological index was introduced by a chemist Harold Wiener in 1947 to calculate the boiling points of paraffins. This numerical representation of a molecular graph has shown to be very useful quantity to use in the quantitative structure-property relationship ($QSPR$) [5]. It has also many applications in communication, facility location, cryptography, etc., that are effectively modeled by a connected graph G with some restrictions [6]. This index was originally defined for trees to correlate the certain physico-chemical properties of alkanes, alcohols, amines and their compounds. Hosoya [15] defined the

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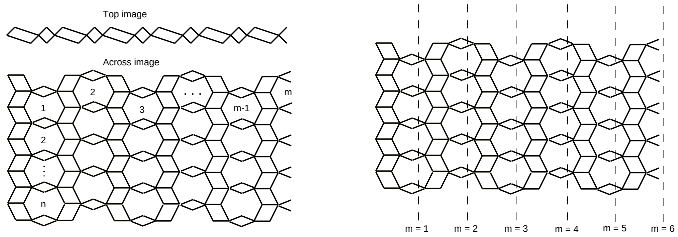

FIGURE 1. The graph of $TiO_2[m,n]$-nanotubes, for $m = 6$ and $n = 4$.

notion of Wiener index for any graph G as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v). \tag{1}$$

Recently, Baig et al. [4] studied the Randic index, atom-bond conenctivity index and geometric-arithmetic index of poly oxide, poly silicate, dominating oxide and dominating silicate networks. Ashrafi et al. [1] studied the PI, Szeged and edge Szeged indices of some nanostar dendrimers. Recently, in [2, 16] some researchers investigated m-order connectivity indices of nanostar dendrimers. The atom-bond connectivity index and geometric-arithmetic index of nanostar dendrimers and some polyomino chains were studied in [14]. The atom-bond conenctivity index and geometric-arithmetic index of some fullerenes was studied in [3]. Rostami et al. [18] studied the first kind of geometric-arithmetic index of some nanostar dendrimers. Ghorbani et al. [9] studied the nullity of an infinite class of nanostar dendrimers. The anti-Kekule number of some nanotubes was studied in [17].

As a well-known semiconductor with a numerous technological applications, Titania is comprehensively studied in materials science. Titania nanotubes were systematically synthesized during the last 10-15 years using different methods and carefully studied as prospective technological materials. The growth mechanism for TiO_2 nanotubes has been well-studied (see [12]). Due to the applications of Titania nanotubes, their comprehensive theoretical studies attract enhanced attention. The TiO_2 sheets with a thickness of a few atomic layers were found to be remarkably stable [8].

The graph of the Titania nanotubes $TiO_2[m,n]$ is presented in Figure 1 where m denotes the number of octagons in a row and n denotes the number of octagons in a column of the Titania nanotube. The next section deals with computation of first versions of atom-bond connectivity index and geometric-arithmetic index of Titanium nanotubes TiO_2.

2. The ABC and GA indices of TiO_2 nanotubes

Let H be a simple connected graph with vertex set $V(H)$ and edge set $E(H)$. The degree d_v of a vertex $v \in V(H)$ is the number of edges incident on v and $S_u = \sum_{v \in N_H(u)} d_v$, where $N_H(u) = \{v \in V(H) \mid uv \in E(H)\}$. Introduced by Estrada et al. [7], the atom-bond connectivity index (ABC-index) is defined by

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

Recently, Ghorbani et al. [10] introduced the fourth version of ABC-index defined by

$$ABC_4(H) = \sum_{uv \in E(H)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}. \tag{3}$$

Another well-known connectivity topological descriptor is the geometric-arithmetic index (GA-index) which was introduced by Vukičević and Furtula [19] and is defined by

$$GA(H) = \sum_{uv \in E(H)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \tag{4}$$

Graovac et al. [11] proposed the fifth version of GA-index which is defined by

$$GA_5(H) = \sum_{uv \in E(H)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}. \tag{5}$$

With each edge uv, we associate two pairs (d_u, d_v) and (S_u, S_v). The edge partition of Titania nanotubes TiO_2 with respect to the degrees of the end-vertices of edges and with respect to the sum of degrees of the neighbours of end-vertices of edges is given by Table 1 and Table 2-3, respectively.

TABLE 1. The (d_u, d_v)-type edge partition of Titania nanotubes.

d_u, d_v	No. of edges
$(2, 4)$	$6n$
$(2, 5)$	$2n + 4mn$
$(3, 4)$	$2n$
$(3, 5)$	$6n(m-1) + 4n$

Theorem 2.1. *Consider the graph of $G \cong TiO_2$ nanotube, then its atom-bond connectivity index is equal to*

$$ABC(G) = n\{(2m+4)\sqrt{2} + \frac{(6m-2)\sqrt{10}}{5} + \frac{\sqrt{15}}{3}\}.$$

Proof. The (d_u, d_v)-type edge partition of the graph G is shown in Table 1. We prove the desired result by using Table 1 and the formula of atom-bond connectivity index given by equation (2) as follows.

$ABC(G) = (6n)\sqrt{\frac{2+4-2}{2\times4}} + (2n+4mn)\sqrt{\frac{2+5-2}{2\times5}} + (2n)\sqrt{\frac{3+4-2}{3\times4}} + (6n(m-1) + 4n)\sqrt{\frac{3+5-2}{3\times5}}$.

After simplification and rearranging the terms, we get

$ABC(G) = n\{(2m+4)\sqrt{2} + \frac{(6m-2)\sqrt{10}}{5} + \frac{\sqrt{15}}{3}\}$. □

Theorem 2.2. *Consider the graph of $G \cong TiO_2$ nanotube, then its geometric arithmetic index is equal to*

$$GA(G) = n\{4\sqrt{2} + \frac{8\sqrt{3}}{7} + \frac{(4+8m)\sqrt{10}}{7} + \frac{(3m-1)\sqrt{15}}{2}\}.$$

Proof. We prove the above result by using Table 1 and the formula of geometric-arithmetic index given by equation (4) as follows.

$GA(G)=(6n)\frac{2\sqrt{2\times4}}{2+4} + (2n+4mn)\frac{2\sqrt{2\times5}}{2+5} + (2n)\frac{2\sqrt{3\times4}}{3+4} + (6n(m-1)+4n)\frac{2\sqrt{3\times5}}{3+5}$.

After simplification and rearranging the terms, we get

$GA(G) = n\{4\sqrt{2} + \frac{8\sqrt{3}}{7} + \frac{(4+8m)\sqrt{10}}{7} + \frac{(3m-1)\sqrt{15}}{2}\}$. □

The next section deals with computation of fourth and fifth versions of atom-bond connectivity index and geometric-arithmetic index (resp.) of Titania nanotubes TiO_2.

3. The ABC_4 and GA_5 indices of TiO_2 nanotubes

For $m > 1$ and n even, the fourth atom-bond connectivity index and fifth arithmetic-geometric index is calculated in the following theorem.

Theorem 3.1. *Consider the graph of $G \cong TiO_2$ nanotube, then its fourth atom bond connectivity index is equal to*

$$ABC_4(G) = n\{\frac{\sqrt{5}}{3}+\sqrt{6}+\frac{2}{\sqrt{7}}+\frac{(2m-1)\sqrt{30}}{5}+\frac{(2m-2)\sqrt{2730}}{65}+\frac{\sqrt{57}}{9}+\frac{10}{\sqrt{182}}+\frac{8}{9}\}.$$

Proof. Consider the graph of $G \cong TiO_2$ nanotube for $m > 1$ and n even. The (S_u, S_v)-type edge-partition for every $m > 1$ and n is even is given in Table 2.

Now, we derive the expression for ABC_4 index for the graph G by using Table 2 and the formula of fourth atom-bond connectivity index given by equation (3) as follows.

$ABC_4(G)=(4n)\sqrt{\frac{8+9-2}{8\times9}}+(2n)\sqrt{\frac{9+9-2}{9\times9}}+(2n)\sqrt{\frac{9+12-2}{9\times12}}+(2n)\sqrt{\frac{9+14-2}{9\times14}}+(4n)\sqrt{\frac{10+12-2}{10\times12}}$

Table 2. The (S_u, S_v)-type edge partition of Titania nanotubes.

S_u, S_v	No. of edges
$(8,9)$	$4n$
$(9,9)$	$2n$
$(9,12)$	$2n$
$(9,14)$	$2n$
$(10,12)$	$4n$
$(10,13)$	$4mn-4n$
$(12,14)$	$2n$
$(12,15)$	$2n$
$(13,14)$	$2n$
$(13,15)$	$6mn-8n$

$+(4mn-4n)\sqrt{\frac{10+13-2}{10\times13}} + (2n)\sqrt{\frac{12+14-2}{12\times14}} + (2n)\sqrt{\frac{12+15-2}{12\times15}} + (2n)\sqrt{\frac{13+14-2}{13\times14}} + (6mn-8n)\sqrt{\frac{13+15-2}{13\times15}}$.

After simplification and rearranging the terms, we get

$ABC_4(G) = n\{\frac{\sqrt{5}}{3} + \sqrt{6} + \frac{2}{\sqrt{7}} + \frac{(2m-1)\sqrt{30}}{5} + \frac{(2m-2)\sqrt{2730}}{65} + \frac{\sqrt{57}}{9} + \frac{10}{\sqrt{182}} + \frac{8}{9}\}$. □

Theorem 3.2. *Consider the graph of $G \cong TiO_2$ nanotube for $m > 1$ and n even, then its fifth geometric-arithmetic index is equal to*

$$GA_5(G) = n\{\frac{48\sqrt{2}}{17} + \frac{8\sqrt{3}}{7} + \frac{8\sqrt{5}}{9} + \frac{12\sqrt{14}}{23} + \frac{8\sqrt{30}}{11} + \frac{(8m-8)\sqrt{130}}{23} + \frac{(3m-4)\sqrt{195}}{7} + \frac{4\sqrt{182}}{27} + \frac{4\sqrt{42}}{13} + 2\}.$$

Proof. We will prove the fifth geometric-arithmetic index for $G \cong TiO_2$ by using Table 2 and equation (5) as follows.

$GA_5(G)=(4n)\frac{2\sqrt{8\times9}}{8+9} + (2n)\frac{2\sqrt{9\times9}}{9+9} + (2n)\frac{2\sqrt{9\times12}}{9+12} + (2n)\frac{2\sqrt{9\times14}}{9+14} + (4n)\frac{2\sqrt{10\times12}}{10+12} + (4mn-4n)\frac{2\sqrt{10\times13}}{10+13} + (2n)\frac{2\sqrt{12\times14}}{12+14} + (2n)\frac{2\sqrt{12\times15}}{12+15} + (2n)\frac{2\sqrt{13\times14}}{13+14} + (6mn-8n)\frac{2\sqrt{13\times15}}{13+15}$.

After simplification and rearranging the terms, we get

$GA_5(G) = n\{\frac{48\sqrt{2}}{17} + \frac{8\sqrt{3}}{7} + \frac{8\sqrt{5}}{9} + \frac{12\sqrt{14}}{23} + \frac{8\sqrt{30}}{11} + \frac{(8m-8)\sqrt{130}}{23} + \frac{(3m-4)\sqrt{195}}{7} + \frac{4\sqrt{182}}{27} + \frac{4\sqrt{42}}{13} + 2\}$. □

For $m > 1$ and n odd, the fourth atom-bond connectivity index and fifth arithmetic-geometric index is calculated in the following theorem.

Theorem 3.3. *Consider the graph of $G \cong TiO_2$ nanotube, then its fourth atom-bond connectivity index is equal to*

$ABC_4(G) = n\{\frac{2\sqrt{5}}{6} + \sqrt{6} + \frac{(2m-1)\sqrt{30}}{5} + \frac{\sqrt{57}}{9} + \frac{8}{9} + \frac{10}{\sqrt{182}} + \frac{(2m-2)\sqrt{2730}}{65} + \frac{2}{\sqrt{7}}\} + m\{\frac{2\sqrt{6}}{13} + \frac{2\sqrt{7}}{15} - \frac{2\sqrt{30}}{15} + \frac{2\sqrt{138}}{15} - \frac{2\sqrt{2730}}{65}\} + \frac{2\sqrt{3}}{7} + \frac{2\sqrt{5}}{11} - \frac{15\sqrt{6}}{13} - \frac{2\sqrt{7}}{15} - \frac{2}{\sqrt{7}} + \frac{\sqrt{77}}{11} + \frac{\sqrt{1862}}{49} - \frac{2\sqrt{138}}{5} + \frac{\sqrt{374}}{11} + \frac{2\sqrt{770}}{35} + \frac{\sqrt{22}}{12} + \frac{\sqrt{26}}{14} + \frac{2\sqrt{2730}}{65} - \frac{8}{9} - \frac{\sqrt{57}}{9} - \frac{\sqrt{30}}{5}.$

Proof. Consider the graph of $G \cong TiO_2$ nanotube for $m > 1$ and n odd. The (S_u, S_v)-type edge-partition for every $m > 1$ and n odd is given in Table 3. Now we derive the ABC_4 formula for the graph G by using Table 3 and the formula of fourth atom-bond connectivity index given by equation (3) as follows.

TABLE 3. The (S_u, S_v)-type edge partition of Titania nanotubes.

Su, Sv	No. of edges
$(7,7)$	1
$(7,14)$	2
$(8,9)$	$4n-4$
$(8,11)$	4
$(9,9)$	$2n-2$
$(9,12)$	$2n-2$
$(9,14)$	$2n-2$
$(10,12)$	$4n-4$
$(10,13)$	$4mn-4n-4(m-1)$
$(10,14)$	4
$(10,15)$	$4m-4$
$(11,11)$	1
$(11,12)$	2
$(12,12)$	1
$(12,14)$	$2n-2$
$(12,15)$	$2n$
$(13,13)$	$m-1$
$(13,14)$	$2n$
$(13,15)$	$6mn-8n-2(m-1)$
$(14,14)$	1
$(15,15)$	$m-1$

$ABC_4(G)=(1)\sqrt{\frac{7+7-2}{7\times7}} + (2)\sqrt{\frac{7+14-2}{7\times14}} + (4n-4)\sqrt{\frac{8+9-2}{8\times9}} + (4)\sqrt{\frac{8+11-2}{8\times11}} + (2n-2)\sqrt{\frac{9+9-2}{9\times9}} + (2n-2)\sqrt{\frac{9+12-2}{9\times12}} + (2n-2)\sqrt{\frac{9+14-2}{9\times14}} + (4n-4)\sqrt{\frac{10+12-2}{10\times12}} + (4mn-4n-4(m-1))\sqrt{\frac{10+13-2}{10\times13}} + (4)\sqrt{\frac{10+14-2}{10\times14}} + (4m-4)\sqrt{\frac{10+15-2}{10\times15}} + (1)\sqrt{\frac{11+11-2}{11\times11}} + (2)\sqrt{\frac{11+12-2}{11\times12}} + (1)\sqrt{\frac{12+12-2}{12\times12}} + (2n-2)\sqrt{\frac{12+14-2}{12\times14}} + (2n)\sqrt{\frac{12+15-2}{12\times15}} + (m-1)\sqrt{\frac{13+13-2}{13\times13}} + (2n)\sqrt{\frac{13+14-2}{13\times14}} + (6mn-8n-2(m-1))\sqrt{\frac{13+15-2}{13\times15}} + (2n-2)\sqrt{\frac{14+14-2}{14\times14}} + (m-1)\sqrt{\frac{15+15-2}{15\times15}}.$

After simplification and rearranging the terms, we get

$ABC_4(G) = n\{\frac{2\sqrt{5}}{6} + \sqrt{6} + \frac{(2m-1)\sqrt{30}}{5} + \frac{\sqrt{57}}{9} + \frac{8}{9} + \frac{10}{\sqrt{182}} + \frac{(2m-2)\sqrt{2730}}{65} + \frac{2}{\sqrt{7}}\} + m\{\frac{2\sqrt{6}}{13} + \frac{2\sqrt{7}}{15} - \frac{2\sqrt{30}}{15} + \frac{2\sqrt{138}}{15} - \frac{2\sqrt{2730}}{65}\} + \frac{2\sqrt{3}}{7} + \frac{2\sqrt{5}}{11} - \frac{15\sqrt{6}}{13} - \frac{2\sqrt{7}}{15} - \frac{2}{\sqrt{7}} + \frac{\sqrt{77}}{11} + \frac{\sqrt{1862}}{49} - \frac{2\sqrt{138}}{5} + \frac{\sqrt{374}}{11} + \frac{2\sqrt{770}}{35} + \frac{\sqrt{22}}{12} + \frac{\sqrt{26}}{14} + \frac{2\sqrt{2730}}{65} - \frac{8}{9} - \frac{\sqrt{57}}{9} - \frac{\sqrt{30}}{5}.$ □

Theorem 3.4. *Consider the graph of $G \cong TiO_2$ nanotube for $m > 1$ and n odd, then its fifth arithmetic-geometric index is equal to*

$GA_5(G) = n\{\frac{48\sqrt{2}}{17} + \frac{8\sqrt{3}}{7} + \frac{8\sqrt{5}}{9} + \frac{12\sqrt{14}}{13} + \frac{8\sqrt{30}}{11} + \frac{4\sqrt{42}}{13} + \frac{4\sqrt{182}}{27} + \frac{(8m-8)\sqrt{130}}{23} + \frac{(3m-4)\sqrt{195}}{7} + 2\} + m\{\frac{8\sqrt{6}}{5} - \frac{8\sqrt{130}}{23} - \frac{\sqrt{195}}{7} + 2\} - \frac{48\sqrt{2}}{17} - \frac{8\sqrt{3}}{7} - \frac{8\sqrt{6}}{5} - \frac{12\sqrt{14}}{23} + \frac{16\sqrt{22}}{19} + \frac{8\sqrt{33}}{23} + \frac{2\sqrt{35}}{3} - \frac{8\sqrt{30}}{11} - \frac{4\sqrt{42}}{13} + \frac{\sqrt{195}}{7} + \frac{8\sqrt{130}}{23} + \frac{4\sqrt{98}}{21}$.

Proof. We will prove the fifth geometric-arithmetic index for the graph G by using Table 3 and the formula for calculating GA_5 index given by equation (5) as follows.

$GA_5(G)=(1)\frac{2\sqrt{7\times7}}{7+7} + (2)\frac{2\sqrt{7\times14}}{7+14} + (4n-4)\frac{2\sqrt{8\times9}}{8+9} + (4)\frac{2\sqrt{8\times11}}{8+11} + (2n-2)\frac{2\sqrt{9\times9}}{9+9} + (2n-2)\frac{2\sqrt{9\times12}}{9+12} + (2n-2)\frac{2\sqrt{9\times14}}{9+14} + (4n-4)\frac{2\sqrt{10\times12}}{10+12} + (4mn-4n-4(m-1))\frac{2\sqrt{10\times13}}{10+13} + (4)\frac{2\sqrt{10\times14}}{10+14} + (4m-4)\frac{2\sqrt{10\times15}}{10+15} + (1)\frac{2\sqrt{11\times11}}{11+11} + (2)\frac{2\sqrt{11\times12}}{11+12} + (1)\frac{2\sqrt{12\times12}}{12+12} + (2n-2)\frac{2\sqrt{12\times14}}{12+14}(2n)\frac{2\sqrt{12\times15}}{12+15} + (m-1)\frac{2\sqrt{13\times13}}{13+13} + (2n)\frac{2\sqrt{13\times14}}{13+14} + (6mn-8n-2(m-1))\frac{2\sqrt{13\times15}}{13+15} + (1)\frac{2\sqrt{14\times14}}{14+14} + (m-1)\frac{2\sqrt{15\times15}}{15+15}$.

After simplification and rearranging the terms, we get

$GA_5(G) = n\{\frac{48\sqrt{2}}{17} + \frac{8\sqrt{3}}{7} + \frac{8\sqrt{5}}{9} + \frac{12\sqrt{14}}{13} + \frac{8\sqrt{30}}{11} + \frac{4\sqrt{42}}{13} + \frac{4\sqrt{182}}{27} + \frac{(8m-8)\sqrt{130}}{23} + \frac{(3m-4)\sqrt{195}}{7} + 2\} + m\{\frac{8\sqrt{6}}{5} - \frac{8\sqrt{130}}{23} - \frac{\sqrt{195}}{7} + 2\} - \frac{48\sqrt{2}}{17} - \frac{8\sqrt{3}}{7} - \frac{8\sqrt{6}}{5} - \frac{12\sqrt{14}}{23} + \frac{16\sqrt{22}}{19} + \frac{8\sqrt{33}}{23} + \frac{2\sqrt{35}}{3} - \frac{8\sqrt{30}}{11} - \frac{4\sqrt{42}}{13} + \frac{\sqrt{195}}{7} + \frac{8\sqrt{130}}{23} + \frac{4\sqrt{98}}{21}$. □

4. Conclusions

This paper deals with some degree based topological indices of an infinite class of Titania nanotubes $TiO_2[m, n]$. In this paper, we study the first and fourth versions of atom-bond connectivity index (ABC-index) introduced by Estrada et al. [7] and Ghorbani et al. [10], respectively.

Moreover, we study first and fifth versions of another well-known connectivity topological descriptor known as the geometric-arithmetic index (GA-index) introduced respectively by Vukičević and Furtula [19] and by Graovac et al. [11].

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