Computing three topological indices for Titania nanotubes TiO$_2$[$m$, $n$]

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Abstract

A numeric quantity which characterizes the whole structure of a graph is called a topological index. The concept of Generalized Zagreb, atom–bond connectivity ($ABC$) and geometric–arithmetic ($GA$) topological indices was established in chemical graph theory based on vertex degrees. Later on, other versions of $ABC$ and $GA$ indices were introduced and some of the versions of these indices are recently designed. In this article, we compute, Generalized Zagreb index $GZ$, fourth version of atom–bond connectivity ($ABC_4$) index and fifth version of geometric–arithmetic ($GA_5$) index for an infinite class of Titania nanotubes TiO$_2$[$m$, $n$].

Keywords: Generalized Zagreb index $GZ$; Fourth atom–bond connectivity $ABC_4$ index; Fifth geometric–arithmetic ($GA_5$) index; Titania nanotubes

1. Introduction

Chemical graph theory is a branch of mathematical chemistry which applies graph theory to the mathematical model of chemical phenomenon. Topological indices is a subtopic of chemical graph theory, which correlates certain physico-chemical properties of the underlying chemical compound. A topological index is a function “$\text{Top}$” from ‘$\Sigma$’ to the set of real numbers, where ‘$\Sigma$’ is the set of finite simple graphs with property that $\text{Top}(G) = \text{Top}(H)$ if both $G$ and $H$ are isomorphic. There is a lot of research which has been done on topological indices of different graph families so far, and is of much importance due to their chemical significance. Topological indices are the mathematical measures which correspond to the structure of any simple finite graph. They are invariant under the graph isomorphisms. The significance of topological indices is usually

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associated with quantitative structures property relationship (QSPR) and quantitative structure activity relationship (QSAR) (see [24]).

A graph can be recognized by a numeric number, a polynomial, a sequence of numbers or a matrix which represents the whole graph, and these representations are aimed to be uniquely defined for that graph. A topological index is a numeric quantity associated with a graph which characterizes the topology of the graph and is invariant under graph automorphism. There are some major classes of topological indices such as distance based topological indices, degree based topological indices and counting related polynomials and indices of graphs. Among these classes degree based topological indices are of great importance and play a vital role in chemical graph theory and particularly in chemistry.

Let $G$ be a molecular graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. We denote the order of $G$ by $|V(G)| = v$. The vertices of $G$ correspond to atoms and an edge between two vertices corresponds to the chemical bond between these vertices. An edge in $E(G)$ with end vertices $u$ and $v$ is denoted by $uv$. A subgraph $H$ of a graph $G$ is any graph with $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. A $(v_1, v_n)$-path on $n$ vertices is denoted by $P_n$ and is defined as a graph with vertex set $\{v_i : 1 \leq i \leq n\}$ and edge set $v_iv_{i+1}$, for $1 \leq i \leq n - 1$. The length of a path $P_n$ is the number of edges in it, that is, $n - 1$. The distance $d(u, v)$ between two vertices $u, v \in V(G)$ is defined as the length of the shortest $(u, v)$-path in $G$.

A graph is said to be $k$-connected if for each pair of vertices $u, v \in V(G)$ there exist $k$ internally disjoint paths from $u$ to $v$. A block is a maximal 2-connected subgraph of a graph.

In this article, $G$ is considered to be simple connected graph with vertex set $V(G)$, edge set $E(G)$, minimum degree $\delta(G)$, maximum degree $\Delta(G)$, degree of vertex $u \in V(G)$ is $d_u$ and

$$S_u = \sum_{v \in N_G(u)} d(v) \quad \text{where } N_G(u) = \{v \in V(G) \mid uv \in E(G)\}.$$ 

The idea of topological index appears from work done by Harold Wiener (see [31]) in 1947 although he was working on boiling point of paraffin. He called this index as Wiener index and then theory of topological index started. The reader can find more information about the Wiener index in [18,19].

The first degree-based connectivity index for graphs developed by using vertex degrees is Randić index [21]. For further study of Randić index of various graph families, see [12,23].

A pair of molecular descriptors known as the First Zagreb index $M_1(G)$ and the Second Zagreb index $M_2(G)$ [13], first appeared in the topological formula for the total $\pi$-energy of conjugated molecules that has been derived in 1972 by I. Gutman and N. Trinajstić [13]. Soon after these indices have been used as branching indices [3,4]. Later the Zagreb indices found applications in QSPR and QSAR studies [5,11].

The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a molecular graph $G$ are respectively defined as

$$M_1(G) = \sum_{uv \in E(G)} [\deg(u) + \deg(v)], \quad M_2(G) = \sum_{uv \in E(G)} [\deg(u) \times \deg(v)].$$

The new multiplicative versions of $M_1(G)$ and $M_2(G)$ indices, denoted by $PM_1(G)$ and $PM_2(G)$ (respectively), were first defined in Ghorbani and Azimi [14]. These indices are defined as follows.

$$PM_1(G) = \prod_{uv \in E(G)} (d_u + d_v), \quad PM_2(G) = \prod_{uv \in E(G)} d(u)d(v).$$

In 2011, A. Iranmanesh and M. Azari [2] introduced the Generalized Zagreb index of a connected graph $G$, based on degree of vertices of $G$ for all $r, s \in N$ as:

$$M_{r,s}(G) = \sum_{uv \in E(G)} (d_u^r d_v^s + d_u^s d_v^r). \quad (1)$$

For more results on Zagreb indices, see [2,17,20,28,30].

The atom–bond connectivity (ABC) index was firstly introduced by Estrada et al. in [6]. Later on the fourth member of the class of $ABC$ index was introduced by M. Ghorbani et al. [9] in the following way:

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_v + S_u - 2}{S_v S_u}}. \quad (2)$$
It is easy to see that

\[ \text{In the molecular graph of TiO}_2 \text{ multiple Zagreb index of TiO}_2 \]

2. Main results

As a well-known semiconductor with 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. Since the growth mechanism for TiO\(_2\) nanotubes is still not well defined, their comprehensive theoretical studies attract enhanced attention. TiO\(_2\) sheets with a thickness of a few atomic layers were found to be remarkably stable [7]. Recently M. A. Malik and M. Imran [16] computed multiple Zagreb index of TiO\(_2\) nanotubes.

The graph of the Titania nanotube TiO\(_2\)[m, n] is presented in Fig. 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.

Let us define the partitions for the vertex set and the edge set of the Titania nanotube TiO\(_2\), for \( \delta(G) \leq k \leq \Delta(G) \), \( 2\delta(G) \leq i \leq 2\Delta(G) \) and \( \delta(G)^2 \leq j \leq \Delta(G)^2 \), then we have

\[ V_k = \{ v \in V(G) \mid \deg(v) = k \}, \quad E_i = \{ e = uv \in E(G) \mid d(u) + d(v) = i \}. \]

In the molecular graph of TiO\(_2\)-nanotube, we can see that \( 2 \leq d(G) \leq 5 \). So, we have the vertex partitions as follows.

\[ V_2 = \{ u \in V(G) \mid d(u) = 2 \}, \quad V_3 = \{ u \in V(G) \mid d(u) = 3 \}. \]

\[ V_4 = \{ u \in V(G) \mid d(u) = 4 \}, \quad V_5 = \{ u \in V(G) \mid d(u) = 5 \}. \]

It is easy to see that \( |V_2| = 2mn + 4n \), \( |V_3| = 2mn \), \( |V_4| = 2n \), \( |V_5| = 2mn \). So we have \( |V(TiO_2)| = 6n(m + 1) \).

Similarly, the edge partitions of the graph TiO\(_2\) are as follows.

\[ E_6 = \{ e = uv \in E(G) \mid d(u) = 2 \& d(v) = 4 \}. \]

\[ E_7 = \{ e = uv \in E(G) \mid d(u) = 2 \& d(v) = 5 \} \]

\[ \cup \{ e = uv \in E(G) \mid d(u) = 3 \& d(v) = 4 \}. \]

\[ E_8 = \{ e = uv \in E(G) \mid d(u) = 3 \& d(v) = 5 \}. \]

The vertex partition \( V_k \) and the edge partitions \( E_i \) are collectively exhaustive, that is

\[ \bigcup_{k=\delta(G)}^{\Delta(G)} V_k = V(G), \quad \bigcup_{i=\delta(G)}^{2\Delta(G)} E_i = E(G). \]
Theorem 2.2. The Generalized Zagreb index $GZ$, of the Titania nanotube $TiO_2[m, n]$ is given by

$$M_{r,s}(TiO_2) = 6n(d_u^2d_v^4 + d_u^4d_v^2) + (4mn + 4n)(d_u^2d_v^5 + d_u^5d_v^2) + (6mn - 2n)(d_u^2d_v^5 + d_u^5d_v^2).$$

Proof. To compute the Generalized Zagreb index $GZ$, of the Titania nanotube $TiO_2[m, n]$, we need an edge partitions based on degrees of end vertices of each edge. So we presented an edge partitions with their cardinalities in Table 1.

Now using Eq. (1) and Table 1, we obtained the required result as follows.

$$M_{r,s}(G) = \sum_{uv \in E(G)} (d_u^r d_v^s + d_u^s d_v^r) = \sum_{uv \in E_6(G)} (d_u^r d_v^s + d_u^s d_v^r) + \sum_{uv \in E_7(G)} (d_u^r d_v^s + d_u^s d_v^r) + \sum_{uv \in E_8(G)} (d_u^r d_v^s + d_u^s d_v^r)$$

$$= |E_6(G)|(d_u^2d_v^4 + d_u^4d_v^2) + |E_7(G)|(d_u^2d_v^5 + d_u^5d_v^2) + |E_8(G)|(d_u^3d_v^5 + d_u^5d_v^3)$$

$$= 6n(d_u^2d_v^4 + d_u^4d_v^2) + (4mn + 4n)(d_u^2d_v^5 + d_u^5d_v^2) + (6mn - 2n)(d_u^3d_v^5 + d_u^5d_v^3).$$

$$\Box$$

In first theorem we computed the Generalized Zagreb index $GZ$, of the Titania nanotube $TiO_2[m, n]$ in the following way.

Theorem 2.1. The Generalized Zagreb index $GZ$, of the Titania nanotube $TiO_2[m, n]$ is given by

$$M_{r,s}(TiO_2) = 6n(d_u^2d_v^4 + d_u^4d_v^2) + (4mn + 4n)(d_u^2d_v^5 + d_u^5d_v^2) + (6mn - 2n)(d_u^3d_v^5 + d_u^5d_v^3).$$

Proof. To compute the Generalized Zagreb index $GZ$, of the Titania nanotube $TiO_2[m, n]$, we need an edge partitions based on degrees of end vertices of each edge. So we presented an edge partitions with their cardinalities in Table 1.

Now using Eq. (1) and Table 1, we obtained the required result as follows.

$$M_{r,s}(G) = \sum_{uv \in E(G)} (d_u^r d_v^s + d_u^s d_v^r)$$

$$=\sum_{uv \in E_6(G)} (d_u^r d_v^s + d_u^s d_v^r) + \sum_{uv \in E_7(G)} (d_u^r d_v^s + d_u^s d_v^r) + \sum_{uv \in E_8(G)} (d_u^r d_v^s + d_u^s d_v^r)$$

$$= |E_6(G)|(d_u^2d_v^4 + d_u^4d_v^2) + |E_7(G)|(d_u^2d_v^5 + d_u^5d_v^2) + |E_8(G)|(d_u^3d_v^5 + d_u^5d_v^3)$$

$$= 6n(d_u^2d_v^4 + d_u^4d_v^2) + (4mn + 4n)(d_u^2d_v^5 + d_u^5d_v^2) + (6mn - 2n)(d_u^3d_v^5 + d_u^5d_v^3).$$

$$\Box$$

$\textbf{Theorem 2.2.}$ The atom–bond connectivity $ABC_4$ index, of the Titania nanotube $TiO_2[m, n]$ is given by

$$ABC_4(TiO_2[m, n]) = \frac{2}{5\sqrt{\frac{13}{2}}} + 2\sqrt{\frac{2}{7}} + 2n\sqrt{\frac{2}{3}} + 2n\sqrt{\frac{5}{6}} + 2m\sqrt{\frac{17}{10}} + 2n\sqrt{\frac{17}{11}} + 2n\sqrt{\frac{5}{13}} + 6n\sqrt{\frac{2}{21}}$$

$$+ (4mn + 2n)\sqrt{\frac{21}{130}} + (2mn - 2n)\sqrt{\frac{2}{13}} + (12mn - 8n)\sqrt{\frac{2}{13}}.$$
\[ + (2n) \sqrt{\frac{10 + 9 - 2}{10 \times 9}} + (6m) \sqrt{\frac{11 + 9 - 2}{11 \times 9}} + (3m) \sqrt{\frac{13 + 9 - 2}{13 \times 9}} + (2n) \sqrt{\frac{7 + 13 - 2}{7 \times 13}} \]
\[ + (4mn + 2n) \sqrt{\frac{10 + 13 - 2}{10 \times 13}} + (2mn - 2n) \sqrt{\frac{11 + 13 - 2}{11 \times 13}} + (6mn - 4n) \sqrt{\frac{13 + 13 - 2}{13 \times 3}} \]
\[ = \frac{2}{5} \sqrt{\frac{13}{2}} + 2 \sqrt{\frac{2}{7}} + \frac{2n \sqrt{2}}{3} + 2n \sqrt{\frac{5}{6}} + \frac{2n}{3} \sqrt{\frac{17}{10}} + 2m \sqrt{\frac{17}{11}} + 2n \sqrt{\frac{5}{13}} + 6n \sqrt{\frac{2}{51}} \]
\[ + (4mn + 2n) \sqrt{\frac{21}{130}} + (2mn - 2n) \sqrt{\frac{2}{13}} + (12mn - 8n) \sqrt{\frac{2}{13}}. \square \]  

**Theorem 2.3.** The geometric–arithmetic \( G_A(T) \) index of Titania nanotube \( TiO_2[m, n] \) is given by

\[ G_A(TiO_2[m, n]) = \frac{4 \sqrt{2}}{3} + \frac{\sqrt{35} \times 3}{3} + \frac{3n \sqrt{7}}{4} + \frac{48n \sqrt{2}}{7} + \frac{12n \sqrt{10}}{19} + \frac{9m \sqrt{11}}{5} + \frac{9m \sqrt{13}}{11} + \frac{n \sqrt{91}}{5} \]
\[ + \frac{(8mn + 4n) \sqrt{103}}{23} + \frac{(mn - n) \sqrt{141}}{6} + (6mn - 4n). \]

**Proof.** To compute the geometric–arithmetic \( G_A(T) \) index of the Titania nanotube \( TiO_2[m, n] \), we need an edge partition of the Titania nanotube \( TiO_2[m, n] \), based on degree sum of neighbors of end vertices of each edge. We presented these partitions with their cardinalities in Tables 2 and 3. Now using Eq. (2) and Tables 2, 3, we obtained the required result as follows.

\[ G_A(T) = \sum_{u \in E(G)} \frac{2 \sqrt{S_u S_{u'}}}{S_u + S_{u'}} \]
\[ = (4) \sqrt{\frac{10 \times 5}{10 + 5}} + (4) \sqrt{\frac{7 \times 5}{7 + 5}} + (4n) \sqrt{\frac{7 \times 9}{7 + 9}} + (8n) \sqrt{\frac{8 \times 9}{8 + 9}} \]
\[ + (4n) \sqrt{\frac{10 \times 9}{10 + 9}} + (12m) \sqrt{\frac{11 \times 9}{11 + 9}} + (6m) \sqrt{\frac{13 \times 9}{13 + 9}} + (4n) \sqrt{\frac{7 \times 13}{7 + 13}} \]
\[ + (8mn + 4n) \sqrt{\frac{10 \times 13}{10 + 13}} + (4mn - 4n) \sqrt{\frac{11 \times 13}{11 + 13}} + (12mn - 8n) \sqrt{\frac{13 \times 13}{13 + 13}} \]
\[ = \frac{4 \sqrt{2}}{3} + \frac{\sqrt{35} \times 4}{3} + \frac{3n \sqrt{7}}{4} + \frac{48n \sqrt{2}}{7} + \frac{12n \sqrt{10}}{19} + \frac{9m \sqrt{11}}{5} + \frac{9m \sqrt{13}}{11} + \frac{n \sqrt{91}}{5} \]
\[ + \frac{(8mn + 4n) \sqrt{103}}{23} + \frac{(mn - n) \sqrt{141}}{6} + (6mn - 4n). \square \]

3. Conclusion and general remarks

In this paper, certain degree based topological indices, namely Generalized Zagreb index \( GZ \), atomic-bond connectivity index \( ABC_4 \) and geometric–arithmetic index \( G_A(T) \) were studied for the first time. To construct and study new architectures/ nanotubes has always been an open problem in both network and art/design sciences. In future, we are interested to design some new architectures/networks and then study their topological indices which will be quite helpful to understand their underlying topologies.

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References


