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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 $TiO_2[m, n]$.
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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 "*Top*" from '$\sum$' to the set of real numbers, where '$\sum$' is the set of finite simple graphs with property that $Top(G) = Top(H)$ 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 $|V(G)| = \nu$. 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 $v_i v_{i+1}$, 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 π-energy of conjugated molecules that has been derived in 1972 by I. Gutman and N. Trinajsti [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:

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

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:

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

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