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Computation of Reduced Zagreb and Multiplicative Reduced Zagreb Indices of Titania Nanotubes

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Abstract. In Chemical Science, the methods of topological index computation can help to find out of biological chemical information of drugs. In this paper, we introduce the multiplicative reduced first Zagreb index, multiplicative reduced modified first Zagreb index and multiplicative reduced F-index of a graph. Also we compute some reduced Zagreb indices and multiplicative reduced indices for titania nanotubes.

Keywords: multiplicative reduced first Zagreb index, multiplicative reduced modified first Zagreb index, multiplicative reduced F-index, titania nanotube.

AMS Mathematics Subject Classification (2010): 05*C*05, 05*C*07, 05*C*90.

1. Introduction

Let G be a finite, simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. For other undefined notations, readers may refer to [1]. Chemical graph theory has an important effect on the development of Chemical Sciences. A single number that can be used to characterize some property of the graph of a molecular is called a topological index for that graph. Numerous such topological indices have been considered in Theoretical Chemistry and have found some applications, especially in QSPR/QSAR research, see [2].

The reduced first Zagreb index [3] of a graph G is defined as

$$RM_1(G) = \sum_{u \in V(G)} \left(d_G(u) - 1\right)^2. \tag{1}$$

Recently, Kulli [4] introduced the reduced modified first Zagreb index, defined as

$${}^{m}RM_1(G) = \sum_{u \in V(G)} \frac{1}{\left(d_G(u) - 1\right)^2}. \tag{2}$$

The reduced F-index [4] of a graph G is defined as

$$RF(G) = \sum_{u \in V(G)} \left(d_G(u) - 1\right)^3. \tag{3}$$

We now introduce the multiplicative reduced first Zagreb index, the multiplicative reduced modified first Zagreb index and multiplicative reduced F-index of a graph as follows:

The multiplicative reduced first Zagreb index of a graph G is defined as

$$RM_1II(G) = \prod_{u \in V(G)} \left(d_G(u) - 1\right)^2. \tag{4}$$

The multiplicative reduced modified first Zagreb index of a graph G is defined as

$$^{m}RM_1II(G) = \prod_{u \in V(G)} \frac{1}{\left(d_G(u) - 1\right)^2}. \tag{5}$$

The multiplicative reduced F-index of a graph G is defined as

$$RFII(G) = \prod_{u \in V(G)} \left(d_G(u) - 1\right)^3. \tag{6}$$

Recently, some reduced topological indices were studied, for example, in [5, 6, 7, 8, 9], and many other multiplicative indices were studied, for example, in [10, 11, 12, 13, 14, 15, 16, 17, 18].

The study of titania nanotubes has received much attention in Chemical and Mathematical literature (see 19, 20). In this paper, the reduced first Zagreb index, multiplicative reduced first Zagreb index, multiplicative reduced modified first Zagreb index and multiplicative reduced F-index for titania nanotubes are determined.

2. Results for titania nanotubes

Titania nanotube is studied in material science. The titania nanotubes denoted by $TiO_2[m,n]$ for $m,n \in N$, where m is the number of octagons C_8 in a row and n is the number of octagons C_8 in a column. The graph of $TiO_2[m,n]$ is presented in Figure 1.

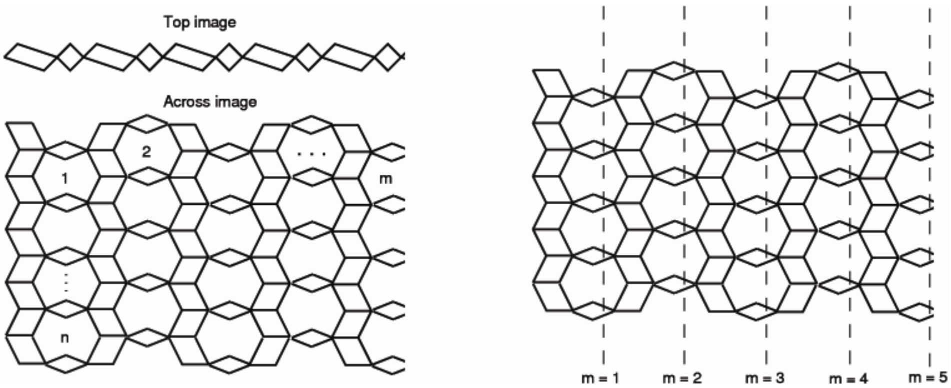

Figure 1: The graph of TiO_2[m, n]-nanotube

Let G be the graph of titania nanotube $TiO_2[m,n]$ with $6n(m+1)$ vertices and $10mn+8n$ edges. In G, by calculation, there are four types of vertices as given in Table 1.

$d_G(u) \backslash u \in V(G)$	2	3	4	5
Number of vertices	$2mn+4n$	$2mn$	$2n$	$2mn$

Table 1: Vertex partition of $TiO_2[m,n]$ nanotubes

Theorem 1. The reduced first Zagreb index of titania nanotubes TiO_2 is

$$RM_1(TiO_2) = 42mn + 22n.$$

Proof: Let $G = TiO_2$. By using equation (1) and from Table 1, we deduce

$$\begin{aligned} RM_1(TiO_2) &= \sum_{u \in V(G)} (d_G(u) - 1)^2 \\ &= (2-1)^2 (2mn+4n) + (3-1)^2 2mn + (4-1)^2 2n + (5-1)^2 2mn \\ &= 42mn + 22n. \end{aligned}$$

Theorem 2. The reduced modified first Zagreb index of titania nanotubes TiO_2 is

$$^m RM_1(TiO_2) = \frac{21}{8} mn + \frac{38}{9} n.$$

Proof: Let $G = TiO_2$. By using equation (2) and from Table 1, we deduce

$$\begin{aligned} {}^m RM_1(TiO_2) &= \sum_{u \in V(G)} \frac{1}{(d_G(u) - 1)^2} \\ &= \frac{1}{(2-1)^2}(2mn+4n) + \frac{1}{(3-1)^2} 2mn + \frac{1}{(4-1)^2} 2n + \frac{1}{(5-1)^2} 2mn \\ &= \frac{21}{8} mn + \frac{38}{9} n. \end{aligned}$$

Theorem 3. The reduced F-index of titania nanotubes TiO_2 is

$$RF(TiO_2) = 146mn + 58n.$$

Proof: Let $G = TiO_2$. By using equation (3) and from Table 1, we derive

$$\begin{aligned} RF(TiO_2) &= \sum_{u \in V(G)} (d_G(u) - 1)^3 \\ &= (2-1)^3 (2mn+4n) + (3-1)^3 2mn + (4-1)^3 2n + (5-1)^3 2mn \\ &= 146mn + 58n. \end{aligned}$$

Theorem 4. The multiplicative reduced first Zagreb index of titania nanotubes TiO_2 is

$$RM_1 II(TiO_2) = 2^{12mn} \times 3^{4n}.$$

Proof: Let $G = TiO_2$. By using equation (4) and from Table 1, we have

$$\begin{aligned} RM_1 II(TiO_2) &= \prod_{u \in V(G)} (d_G(u) - 1)^2 \\ &= (2-1)^{2(2mn+4n)} \times (3-1)^{2(2mn)} \times (4-1)^{2(2n)} \times (5-1)^{2(2mn)} \\ &= 2^{12mn} \times 3^{4n}. \end{aligned}$$

Theorem 5. The multiplicative reduced modified first Zagreb index of titania nanotubes TiO_2 is

$$ {}^{m}RM_1II\left(TiO_2\right)=\left(\frac{1}{2}\right)^{12mn}\times\left(\frac{1}{3}\right)^{4n}. $$

Proof: Let $G = TiO_2$. By using equation (5) and from Table 1, we deduce

$$ {}^{m}RM_1II\left(TiO_2\right)=\prod_{u\in V(G)}\frac{1}{\left(d_G(u)-1\right)^2} $$

$$ =\left[\frac{1}{(2-1)^2}\right]^{2mn+4n}\times\left[\frac{1}{(3-1)^2}\right]^{2mn}\times\left[\frac{1}{(4-1)^2}\right]^{2n}\times\left[\frac{1}{(5-1)^2}\right]^{2mn} $$

$$ =\left(\frac{1}{2}\right)^{12mn}\times\left(\frac{1}{3}\right)^{4n}. $$

Theorem 6. The multiplicative reduced F-index of titania nanotubes TiO_2 is

$$ RFII\left(TiO_2\right)=2^{18mn}\times 3^{6n}. $$

Proof: Let $G = TiO_2$. By using equation (6) and from Table 1, we obtain

$$ RFII\left(TiO_2\right)=\prod_{u\in V(G)}\left(d_G(u)-1\right)^3 $$

$$ =(2-1)^{3(2mn+4n)}\times(3-1)^{3(2mn)}\times(4-1)^{3(2n)}\times(5-1)^{3(2mn)} $$

$$ =2^{18mn}\times 3^{6n}. $$

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