

Computation of Multiplicative Minus F -indices of Titania Nanotubes

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Abstract. A titania nanotube is studied in material science. In this study, we introduce the multiplicative square minus F -index, multiplicative modified minus F -index, multiplicative minus connectivity F -index, multiplicative reciprocal minus connectivity F -index and general multiplicative minus F -index of a graph. We compute these multiplicative F -indices for titania nanotubes.

Keywords: multiplicative square minus F -index, multiplicative minus connectivity F -index, general multiplicative minus F -index, titania nanotube.

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1. Introduction

A molecular graph is a graph whose vertices correspond to the atoms and the edges to the bonds. Chemical Graph Theory has an important effect on the development of Chemical Sciences. In Chemistry, topological indices are used for studying QSPR/QSAR, see [1, 2, 3].

We consider only finite, simple, connected graph. Let G be a such graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertices the number of vertices adjacent to u . We refer the book [4] for undefined definitions and notations,

In [5], Furtula et al. defined the F_1 -index as

$$F_1(G) = \sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2],$$

In [6], Kulli defined the F_2 -index as

$$F_2(G) = \sum_{uv \in E(G)} d_G(u)^2 d_G(v)^2.$$

Recently some novel variants of F -indices were introduced and studied such as minus F -indices [7], connectivity F -indices [8], multiplicative F -indices [9], multiplicative first F -index [9, 10].

The multiplicative minus index of a graph was introduced by Kulli in [12], defined as

$$M_{\Pi}(G) = \prod_{uv \in E(G)} |d_G(u) - d_G(v)|.$$

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In [13], Jahanbani et al. defined the multiplicative nano Zagreb index of a graph as

$$NZII(G) = \prod_{uv \in E(G)} |d_G(u)^2 - d_G(v)^2|.$$

In [14], Kulli introduced the square F -index of a graph G and it is defined as

$$QF(G) = \prod_{uv \in E(G)} [d_G(u)^2 - d_G(v)^2].$$

Motivated by the definition of the forgotten topological index and its wide applications, we introduce the following multiplicative F -indices:

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

$$QFII(G) = \prod_{uv \in E(G)} [d_G(u)^2 - d_G(v)^2]^2.$$

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

$${}^m MFII(G) = \prod_{uv \in E(G)} \frac{1}{|d_G(u)^2 - d_G(v)^2|}.$$

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

$$MF_c II(G) = \prod_{uv \in E(G)} \frac{1}{\sqrt{|d_G(u)^2 - d_G(v)^2|}}.$$

The multiplicative reciprocal minus connectivity F -index of a graph G is defined as

$$RMF_c II(G) = \prod_{uv \in E(G)} \sqrt{|d_G(u)^2 - d_G(v)^2|}.$$

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

$$MF^a II(G) = \prod_{uv \in E(G)} [d_G(u)^2 - d_G(v)^2]^a.$$

Recently some multiplicative indices were studied, for example, in [15, 16, 17, 18, 19, 20, 21, 22].

A study of titania nanotubes has received much attention in Chemical and Mathematical literature, see [23, 24, 25]. In this paper, the multiplicative minus F -indices for titania nanotubes are computed.

2. Titania nanotubes

Titania nanotube is studied in material science. The family of titania nanotubes is denoted by $TiO_2[m, n]$, 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 molecular structure of $TiO_2[m, n]$ is depicted in Figure 1.

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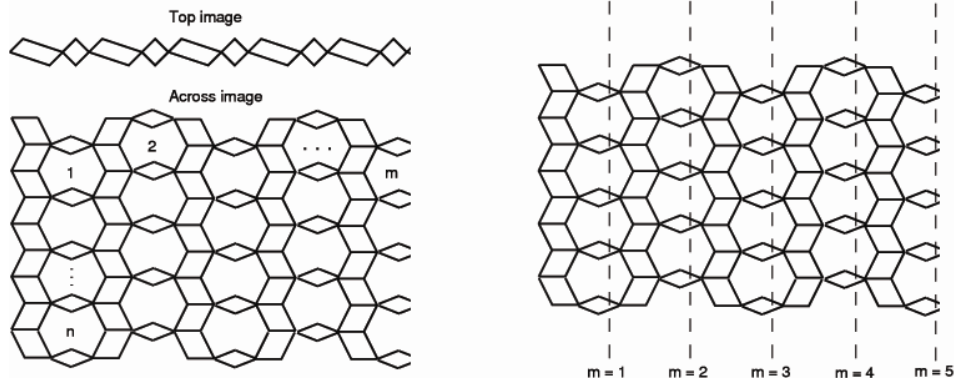


Figure 1: Molecular graph of $TiO_2[m, n]$

Let G be the molecular structure of titania nanotube $TiO_2[m, n]$. The graph G has $6n(m+1)$ vertices and $10mn+8n$ edges. By calculation, we find that G has four types of edges based on the degree of end vertices of each edge as given in Table 1.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(2, 4)	(2, 5)	(3, 4)	(3, 5)
Number of edges	$6n$	$4mn+2n$	$2n$	$6mn-2n$

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

We compute the multiplicative nano Zagreb index of $TiO_2[m, n]$.

Theorem 1. The multiplicative nano Zagreb index of a titania nanotube is

$$NZII(TiO_2) = 12^{6n} \times 21^{4mn+6n} \times 7^{2n} \times 16^{6mn-2n}.$$

Proof: Let G be the graph of TiO_2 . By using definition and Table 1, we deduce

$$\begin{aligned}
 NZII(TiO_2) &= \prod_{uv \in E(G)} |d_G(u)^2 - d_G(v)^2| \\
 &= (|2^2 - 4^2|)^{6n} \times (|2^2 - 5^2|)^{4mn+2n} \\
 &\quad \times (|3^2 - 4^2|)^{2n} \times (|3^2 - 5^2|)^{6mn-2n}. \\
 &= 12^{6n} \times 21^{4mn+2n} \times 7^{2n} \times 16^{6mn-2n}.
 \end{aligned}$$

We compute the multiplicative square minus F -index of $TiO_2[m, n]$.

Theorem 2. The multiplicative square minus F -index of a titania nanotube TiO_2 is

$$QFII(TiO_2) = 12^{12n} \times 21^{8mn+4n} \times 7^{4n} \times 16^{12mn-4n}.$$

Proof: By using definition and Table 1, we derive

$$\begin{aligned}
 QFII(TiO_2) &= \prod_{uv \in E(G)} [d_G(u)^2 - d_G(v)^2]^2 \\
 &= (|2^2 - 4^2|)^{2 \times 6n} \times (|2^2 - 5^2|)^{2(4mn+2n)} \\
 &\quad \times (|3^2 - 4^2|)^{2 \times 2n} \times (|3^2 - 5^2|)^{2(6mn-2n)}. \\
 &= 12^{12n} \times 21^{8mn+4n} \times 7^{4n} \times 16^{12mn-4n}.
 \end{aligned}$$

We determine the multiplicative modified minus F -index of $TiO_2[m, n]$.

Theorem 3. The multiplicative modified minus F -index of $TiO_2[m, n]$ is

$${}^m MFII(TiO_2) = \left(\frac{1}{12}\right)^{6n} \times \left(\frac{1}{21}\right)^{4mn+6n} \times \left(\frac{1}{7}\right)^{2n} \times \left(\frac{1}{16}\right)^{6mn-2n}.$$

Proof: Using definition and Table 1, we obtain

$$\begin{aligned} {}^m MFII(TiO_2) &= \prod_{uv \in E(G)} \frac{1}{|d_G(u)^2 - d_G(v)^2|} \\ &= \left(\frac{1}{|2^2 - 4^2|}\right)^{6n} \times \left(\frac{1}{|2^2 - 5^2|}\right)^{4mn+2n} \\ &\quad \times \left(\frac{1}{|3^2 - 4^2|}\right)^{2n} \times \left(\frac{1}{|3^2 - 5^2|}\right)^{6mn-2n}. \\ &= \left(\frac{1}{12}\right)^{6n} \times \left(\frac{1}{21}\right)^{4mn+6n} \times \left(\frac{1}{7}\right)^{2n} \times \left(\frac{1}{16}\right)^{6mn-2n}. \end{aligned}$$

In the following theorem, we compute the multiplicative minus connectivity F -index of a titania nanotube TiO_2 .

Theorem 4. The multiplicative minus connectivity F -index of TiO_2 is

$$MF_C II(TiO_2) = \left(\frac{1}{12}\right)^{3n} \times \left(\frac{1}{21}\right)^{2mn+n} \times \left(\frac{1}{7}\right)^n \times \left(\frac{1}{16}\right)^{3mn-2n}.$$

Proof: By using definition and Table 1, we have

$$\begin{aligned} MF_C II(TiO_2) &= \prod_{uv \in E(G)} \frac{1}{\sqrt{|d_G(u)^2 - d_G(v)^2|}} \\ &= \left(\frac{1}{\sqrt{|2^2 - 4^2|}}\right)^{6n} \times \left(\frac{1}{\sqrt{|2^2 - 5^2|}}\right)^{4mn+2n} \\ &\quad \times \left(\frac{1}{\sqrt{|3^2 - 4^2|}}\right)^{2n} \times \left(\frac{1}{\sqrt{|3^2 - 5^2|}}\right)^{6mn-2n}. \\ &= \left(\frac{1}{12}\right)^{3n} \times \left(\frac{1}{21}\right)^{2mn+n} \times \left(\frac{1}{7}\right)^n \times \left(\frac{1}{16}\right)^{3mn-2n}. \end{aligned}$$

In the following theorem, we compute the multiplicative minus connectivity F -index of TiO_2 .

Theorem 5. The multiplicative reciprocal minus connectivity F -index of TiO_2 is

$$RMF_C II(TiO_2) = 12^{3n} \times 21^{2mn+n} \times 7^n \times 16^{3mn-2n}.$$

Proof: By using definition and Table 1, we have

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$$\begin{aligned}
 RMF_c II(TiO_2) &= \prod_{uv \in E(G)} \sqrt{|d_G(u)^2 - d_G(v)^2|} \\
 &= \left(\sqrt{|2^2 - 4^2|}\right)^{6n} \times \left(\sqrt{|2^2 - 5^2|}\right)^{4mn+2n} \\
 &\times \left(\sqrt{|3^2 - 4^2|}\right)^{2n} \times \left(\sqrt{|3^2 - 5^2|}\right)^{6mn-2n} \\
 &= 12^{3n} \times 21^{2mn+n} \times 7^n \times 16^{3mn-n}
 \end{aligned}$$

In the next theorem, we compute the general multiplicative minus F -index of TiO_2 .

Theorem 6. The general multiplicative minus F -index of a titania nanotube is

$$MF^a II(TiO_2) = 12^{6an} \times 21^{a(4mn+2n)} \times 7^{2an} \times 16^{a(6mn-2n)}.$$

Proof: By using definition and Table 1, we deduce

$$\begin{aligned}
 MF^a II(TiO_2) &= \prod_{uv \in E(G)} \left[|d_G(u)^2 - d_G(v)^2|\right]^a \\
 &= \left(|2^2 - 4^2|\right)^{a \times 6n} \times \left(|2^2 - 5^2|\right)^{a(4mn+2n)} \\
 &\times \left(|3^2 - 4^2|\right)^{a \times 2n} \times \left(|3^2 - 5^2|\right)^{a(6mn-2n)} \\
 &= 12^{6an} \times 21^{a(4mn+2n)} \times 7^{2an} \times 16^{a(6mn-2n)}.
 \end{aligned}$$

3. Conclusion

In this paper, we have introduced the multiplicative square minus F -index, multiplicative modified minus F -index, multiplicative minus connectivity F -index, multiplicative reciprocal minus connectivity F -index, general minus F -index of a graph. We have computed these newly defined multiplicative minus F -indices for titania nanotubes.

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