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# Computation of Some Minus Indices of Titania Nanotubes

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**Abstract:** A titania nanotube is studied in material science. In this paper, we introduce the modified minus index, minus connectivity index, reciprocal minus connectivity index and general minus index of a graph. We compute these minus topological indices for titania nanotubes.

**MSC:** 05C05, 05C07, 05C12, 05C90.

**Keywords:** Modified minus index, minus connectivity index, reciprocal minus connectivity index, general minus index, titania nanotube.



## 1. Introduction

We consider only finite, connected simple graph $G$ with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex $v$ is the number vertices adjacent to $v$. We refer to [1] for undefined term and notation. Chemical Graph Theory is a branch of Mathematical Chemistry which has an important effect on the development of Chemical Sciences. Several topological indices have been considered in Theoretical Chemistry, see [2]. In [3], Albertson introduced the irregularity index as

$$Alb(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)| \tag{1}$$

Motivated by the definition of the irregularity index, (now we call as minus index denoted by $M_i(G)$), we introduce the modified minus index, minus connectivity index, reciprocal minus connectivity index and general minus index of a graph as follows. The modified minus index of a graph G is defined as

$$^{m}M_i(G) = \sum_{uv \in E(G)} \frac{1}{|d_G(u) - d_G(v)|} \tag{2}$$

The minus connectivity index of a graph G is defined as

$$Mic(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{|d_G(u) - d_G(v)|}} \tag{3}$$

The reciprocal minus, index of a graph G is defined as

$$RMic(G) = \sum_{uv \in E(G)} \sqrt{|d_G(u) - d_G(v)|} \tag{4}$$

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The general minus index of a graph $G$ is defined as

$$M_i^a(G) = \sum_{uv \in E(G)} [|d_G(u) - d_G(v)|]^a \tag{5}$$

where $a$ is a real number. Recently, some new topological indices were studied, for example, in [4–20]. A study of titania nanotubes has received much attention in Mathematical and Chemical literature (see [21–23]). In this paper, we compute the minus index, modified minus index, minus connectivity index, reciprocal minus connectivity index and general minus index for titania nanotuabes.

## 2. Titania Nanotubes

Titania is studied in material science. The titania nanotubes denoted by $TiO_2[m,n]$ for any $m, n \in N$, in which $m$ 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.

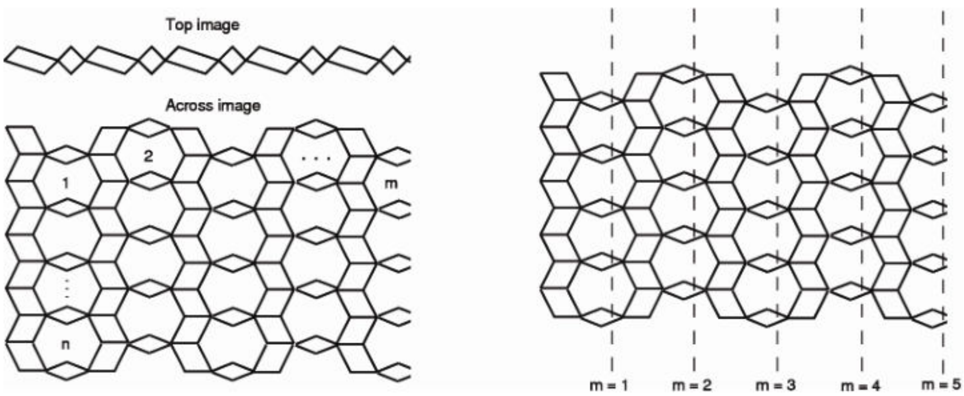


Figure 1: The graph of $TiO_2[m,n]$ nanotube

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 edges based on the degree of end vertices of each edge as given in Table 1.

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

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

In the following theorem, we compute the minus index of titania nanotubes $TiO_2[m,n]$.

**Theorem 2.1.** *The minus index of $TiO_2[m,n]$ nanotubes is $M_i(TiO_2) = 24mn + 16n$.*

*Proof.* Let $G = TiO_2[m,n]$ be the graph of titania nanotube. By using equation (1) and Table 1, we have

$$\begin{aligned} M_i(TiO_2) &= \sum_{uv \in E(G)} |d_G(u) - d_G(v)| \\ &= |2-4|6n + |2-5|(4mn+2n) + |3-4|2n + |3-5|(6mn-2n) \\ &= 24mn + 16n. \end{aligned}$$

□

In the following theorem, we compute the modified minus index of titania nanotubes $TiO_2[m,n]$.

**Theorem 2.2.** *The modified minus index of $TiO_2[m,n]$ nanotubes is*

$$^{m}M_i(TiO_2) = \frac{13}{3}mn + \frac{14}{3}n.$$

*Proof.* Let $G = TiO_2[m,n]$ be the graph of titania nanotube. By using equation (1) and Table 1, we obtain

$$\begin{aligned} ^{m}M_i(TiO_2) &= \sum_{uv\in E(G)} \frac{1}{|d_G(u) - d_G(v)|} \\ &= \left(\frac{1}{|2-4|}\right)6n + \left(\frac{1}{|2-5|}\right)(4mn+2n) + \left(\frac{1}{|3-4|}\right)2n + \left(\frac{1}{|3-5|}\right)(6mn-2n) \\ &= \frac{13}{3}mn + \frac{14}{3}n. \end{aligned}$$

□

In the following theorem, we determine the minus connectivity index of titania nanotubes $TiO_2[m,n]$.

**Theorem 2.3.** *The minus connectivity index of $TiO_2[m,n]$ nanotubes is*

$$Mic(G) = \left(\frac{4}{\sqrt{3}} + \frac{6}{\sqrt{2}}\right)mn + \left(\frac{4}{\sqrt{2}} + \frac{2}{\sqrt{3}} + 2\right)n.$$

*Proof.* Let $G = TiO_2[m,n]$ be the graph of titania nanotube. By using equation (3) and Table 1, we deduce

$$\begin{aligned} Mic(TiO_2) &= \sum_{uv\in E(G)} \frac{1}{\sqrt{|d_G(u) - d_G(v)|}} \\ &= \left(\frac{1}{\sqrt{|2-4|}}\right)6n + \left(\frac{1}{\sqrt{|2-5|}}\right)(4mn+2n) + \left(\frac{1}{\sqrt{|3-4|}}\right)2n + \left(\frac{1}{\sqrt{|3-5|}}\right)(6mn-2n) \\ &= \left(\frac{4}{\sqrt{3}} + \frac{6}{\sqrt{2}}\right)mn + \left(\frac{4}{\sqrt{2}} + \frac{2}{\sqrt{3}} + 2\right)n. \end{aligned}$$

□

In the following theorem, we determine the reciprocal minus connectivity index of titania nanotubes $TiO_2[m,n]$.

**Theorem 2.4.** *The reciprocal minus connectivity index of $TiO_2[m,n]$ nanotubes is*

$$RMic(TiO_2) = \left(4\sqrt{3} + 6\sqrt{2}\right)mn + \left(4\sqrt{2} + \sqrt{3} + 2\right)n.$$

*Proof.* Let $G = TiO_2[m,n]$ be the graph of titania nanotube. By using equation (4) and Table 1, we deduce

$$\begin{aligned} RMic(TiO_2) &= \sum_{uv\in E(G)} \sqrt{|d_G(u) - d_G(v)|} \\ &= \sqrt{|2-4|}6n + \sqrt{|2-5|}\,(4mn+2n) + \sqrt{|3-4|}2n + \sqrt{|3-5|}\,(6mn-2n) \\ &= (4\sqrt{3} + 6\sqrt{2})mn + \left(4\sqrt{2} + \sqrt{3} + 2\right)n. \end{aligned}$$

□

In the following theorem, we complete the general minus index of titania nanotubes $TiO_2[m,n]$.

**Theorem 2.5.** *The general minus index of $TiO_2[m,n]$ nanotubes is*

$$M_i^a(TiO_2) = (4\times 3^a + 6\times 2^a)\,mn + (4\times 2^a + 2\times 3^a + 2)\,n.$$

*Proof.* Let $G = TiO_2[m, n]$ be the graph of titania nanotube. By using equation (5) and Table 1, we obtain

$$\begin{aligned} M_i^a(TiO_2) &= \sum_{uv \in E(G)} [|d_G(u) - d_G(v)|]^a \\ &= (|2-4|)^a\, 6n + (|2-5|)^a\, (4mn+2n) + (|3-4|)^a\, 2n + (|3-5|)^a\, (6mn-2n) \\ &= (4 \times 3^a + 6 \times 2^a)\, mn + (4 \times 2^a + 2 \times 3^a + 2)\, n. \end{aligned}$$

□

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