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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.

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

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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.

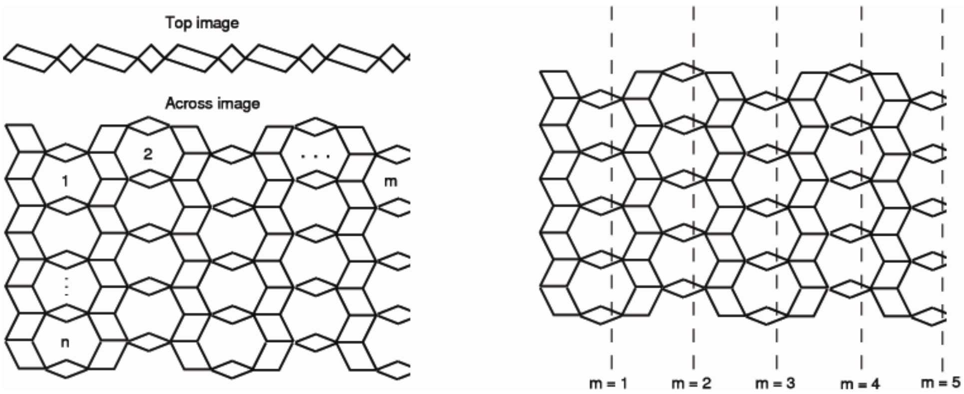

Figure 1: The graph of $TiO_2[m, n]$ nanotube

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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