



# 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

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

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

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

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

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

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

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

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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 nanotubes.

## 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.

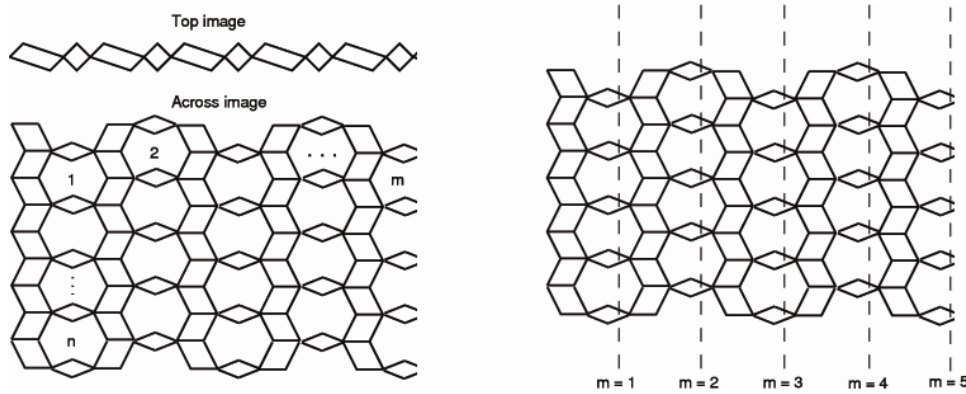


Figure 1: The graph of  $TiO_2[m, n]$  nanotube

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.

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

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

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

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

□

## References

- [1] V.R.Kulli, *Collegiate Graph Theory*, Vishwa International Publications, Gulbarga, India, (2012).
- [2] R.Todeschini and V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley-VCH, Weinheim, (2009).
- [3] M.O.Albertson, *The irregularity of a graph*, Ars. Combin., 46(1997), 219-225.
- [4] B.Furtula and I.Gutman, *A forgotten topological index*, J. Math. Chem., 53(2015), 1184-1190.
- [5] B.Furtula, I.Gutman and S.Ediz, *On difference of Zagreb indices*, Discrete Appl. Math., 178(2014), 83-88.
- [6] V.R.Kulli, *On K indices of graphs*, Int. J. Fuzzy Mathematical Archive, 10(2)(2016), 105-109.
- [7] V.R.Kulli, *Two new arithmetic-geometric ve-degree indices*, Annals of Pure and Applied Mathematics, 17(1)(2018), 107-112.
- [8] V.R.Kulli, *K-edge index of some nanostructures*, Journal of Computer and Mathematical Sciences, 7(7)(2016), 373-378.
- [9] V.R.Kulli, *On K Banhatti indices and K hyper-Banhatti indices of V-Phenylenic nanotubes and nanotorus*, Journal of Computer and Mathematical Sciences, 7(6)(2016), 302-307.
- [10] V. R.Kulli, *General topological indices of circumcoronene series of benzenoid*, International Research Journal of Pure Algebra, 7(5)(2017), 748-753.
- [11] V.R.Kulli, *Computing Banhatti indices of networks*, International Journal of Advances in Mathematics, 2018(1)(2018), 31-40.
- [12] V.R.Kulli, *Some new fifth multiplicative Zagreb indices of PAMAM dendrimers*, Journal of Global Research in Mathematics, 5(2)(2018), 82-86.
- [13] V.R.Kulli, *Multiplicative connectivity Banhatti indices of dendrimer nanostars*, Journal of Chemistry and Chemical Sciences, 8(6)(2018), 964-973.
- [14] V.R.Kulli, *Connectivity Revan indices of chemical structures in drugs*, International Journal of Engineering Sciences and Research Technology, 7(5)(2018), 11-16.
- [15] V.R.Kulli, *Computing the F-ve-degree index and its polynomial of dominating oxide and regular triangulate oxide networks*, International Journal of Fuzzy Mathematical Archive, 16(1)(2018), 1-6.
- [16] V.R.Kulli, *Computation of F-reverse and modified reverse indices of some nanostructures*, Annals of Pure and Applied Mathematics, 18(1)(2018), 37-43.
- [17] V.R.Kulli and M.H.Akhbari, *Multiplicative atom bond connectivity and multiplicative geometric-arithmetic indices of dendrimer nanostars*, Annals of Pure and Applied Mathematics, 16(2)(2018), 429-436.
- [18] A.Milicevic, S. Nikolic and N. Trinajstic, *On reformulated Zagreb indices*, Molecular Diversity, 8(2004), 393-399.
- [19] G.H.Shirdel, H.Rezapour and A.M.Sayadi, *The hyper-Zagreb index of graph operations*, Iranian J. Math. Chem., 4(2)(2013), 213-220.
- [20] B.Zhou and N.Trinajstic, *On a novel connectivity index*, J. Math. Chem., 46(2009), 1252-1270.

- [21] N.De, *On molecular topological properties of  $TiO_2$  nanotubes*, Journal of Nanoscience, (2016), Article ID 1028031, 5 pages.
- [22] V.R.Kulli, *Computation of general topological indices for titania nanotubes*, International Journal of Mathematical Archive, 7(12)(2016), 33-38.
- [23] V.R.Kulli, *Computation of some Gourava indices of titania nanotubes*, International Journal of Fuzzy Mathematical Archive, 12(2)(2017), 75-81.