

Short communication

About the Randić Connectivity, Modify Randić Connectivity and Sum-connectivity Indices of Titania Nanotubes $TiO_2(m,n)$

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Abstract

The Randić Connectivity Index $R(G)$ is one of the oldest connectivity index, introduced by Randić in 1975. Another connectivity indices is the Sum-Connectivity Index $X(G)$ introduced in 2008 by Zhou and Trinajstić. Recently in 2011, a modification of the Randić Connectivity Index of a graph G was introduced by Dvorak et al. In this paper, we compute these connectivity topological indices for a family of molecular graphs known as titania nanotubes $TiO_2(m,n)$.

Keywords: Molecular graph, Nanotubes, Titania nanotubes $TiO_2(m,n)$, Topological indices, Randić index, Sum-connectivity index, Modify Randić index, Zagreb index, Multiple Zagreb index.

1. Introduction

A graph is a collection of points and lines connecting a subset of them. The points and lines in a graph are respectively called vertices and edges of the graph. An edge in $E(G)$ with end vertices u and v is denoted by uv . Two vertices u and v are said to be adjacent if there is an edge between them. In chemical graph theory, the vertices of molecular graph G correspond to the atoms and its edges correspond to the chemical bonds. We denoted the order and size and degree of a vertex/atom v of a molecular graph G by $|V(G)|$, $|E(G)|$ and dv , respectively. The set of all vertices adjacent to a vertex v in $V(G)$ is said to be the neighborhood of v , denoted as $N(v)$. The number of vertices in $N(v)$ is said to be the degree of v . The minimum and maximum vertex degrees in a graph G denoted by $\delta(G)$ and $\Delta(G)$, respectively and are defined as $\min\{dv \mid v \in V(G)\}$ and $\max\{dv \mid v \in V(G)\}$, respectively. Our notation is standard and mainly taken from standard books of chemical graph theory.^{1–3}

We have many connectivity topological indices, for an arbitrary graph with connected structure in chemical

graph theory. The oldest of them is Randić Connectivity Index which has shown to reflect molecular branching, introduced by Milan Randić in 1975,⁴ and defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}, \quad (1)$$

where, d_u and d_v are the degrees of the vertices u and v , respectively.

Another connectivity indices is the Sum-Connectivity Index that was introduced by Zhou and Trinajstić in 2008.^{5,6} The sum-connectivity index $X(G)$ is defined as the sum over all edges of the graph of the terms $(d_u + d_v)^{-2/2}$ and is equal to

$$X(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}, \quad (2)$$

Recently in 2011, Dvorak et al. introduced a modification of the Randić Connectivity Index of G and is defined as

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{\max\{d_u, d_v\}}, \quad (3)$$

that is more tractable from computational point of view. It is much easier to compute Modify Randić index $R'(G)$ than Randić index $R(G)$ (see⁷ for more details). Some basic properties of these indices can be found in the recent letters. For more study, see reference.^{8–13}

In this paper, we investigate the topological Connectivity indices, and compute some formulas for the Randić, Sum-Connectivity and Modify Randić indices of a family of molecular graphs that called titania nanotubes $TiO_2(m,n)$ for positive integers n, m (see Figure 1).

2. Main results and Discussion

In this section, we compute the Randić, Sum-connectivity and Modify Randić Indices for the titania nanotubes $TiO_2(m,n)$ ($\forall m, n \in \mathbb{N}$). Titania nanotubes were systematically synthesized during the last 10–15 years using different methods and carefully studied as prospective technological materials. Since the growth mechanism for TiO_2 Nanotubes is still not well defined, their comprehensive theoretical studies attract enhanced attention. The TiO_2 sheets with a thickness of a few atomic layers were found to be remarkably stable.^{14–17} Molecular graphs titania $TiO_2(m,n)$ is a family of nanotubes, such that the structure of this family of nanotubes consist of the cycles with length four C_4 and eight C_8 . Several topological indices of titania nanotubes (TiO_2) have been studied in the literature.^{18–20}

Let us denote the number of Octagons or cycles C_8 in the first row and column of the 2- Dimensional lattice of TiO_2 nanotubes (Figure 1) by m and n , respectively.

Theorem 1. Let $TiO_2(m,n)$ be the titania nanotubes for positive integers m, n . Then the following indices are calculated by formulas:

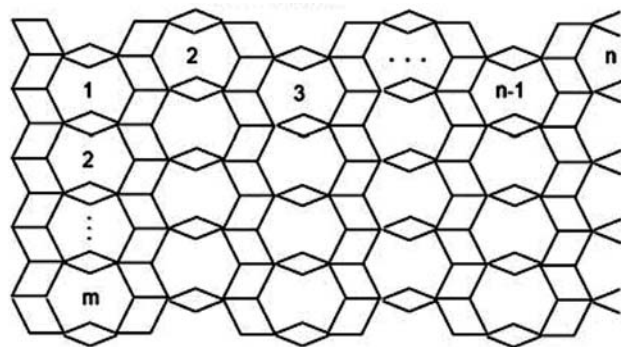


Figure 1. A 2-Dimensional Lattice of the titania nanotubes $TiO_2(m,n)$ ($\forall m, n \in \mathbb{N}$).¹⁷

– The Randić Connectivity index

$$R(TiO_2(m,n)) = \left[\frac{2(\sqrt{15} + \sqrt{10})}{5} m + \left(\frac{45\sqrt{2} + 3\sqrt{10} + 5\sqrt{3} + 2\sqrt{15}}{15} \right) n \right] \quad (4)$$

– The Sum-Connectivity index

$$X(TiO_2(m,n)) = \left[\left(\frac{3\sqrt{2}}{2} + \frac{4\sqrt{7}}{7} \right) m + \left(\sqrt{6} + \frac{4\sqrt{7}}{7} - \frac{\sqrt{2}}{2} \right) n \right] \quad (5)$$

– The Modify Randić index

$$R'(TiO_2(m,n)) = 2n(m+1). \quad (6)$$

Before we prove the main results, let us introduce some definitions.

Definition 1. Consider the graph $G = (V, E)$, then we divide the vertex set $V(G)$ and edge set $E(G)$ of G into several partitions based on the degrees of vertices/atoms in G as follows.⁹

$$\begin{aligned} \forall k: \delta \leq k \leq \Delta, V_k &= \{v \in V(G) | d_v = k\} \\ \forall i: 2\delta \leq i \leq 2\Delta, E_i &= \{uv \in E(G) | d_u + d_v = i\} \\ \forall j: \delta^2 \leq j \leq \Delta^2, E_j^* &= \{uv \in E(G) | d_u \times d_v = j\}. \\ \forall f: \delta \leq f \leq \Delta, E_f^+ &= \{uv \in E(G) | \text{Max}\{d_u, d_v\} = f\} \\ \forall g: \delta \leq g \leq \Delta, E_g^\times &= \{uv \in E(G) | \text{Min}\{d_u, d_v\} = g\}, \end{aligned} \quad (7)$$

Where $d_u (1 \leq d_v \leq n-1)$ be the degrees of $v \in V(G)$ and δ and Δ are the minimum and maximum, respectively.

In particular, let $G = (V, E)$ be a connected molecular graph or nanotubes, then we can divide the vertex set and edge set of G in following partitions:

$$V_i = \{v \in V(G) | d_v = i\}, \forall i = 1, 2, \dots, 5 \quad (8)$$

Since the degree of an atom (or vertex) of the molecular graph is equal to 1, 2, ..., 5 and the hydrogen atoms (with degree 1) in G are often omitted.

In particular, let $TiO_2(m,n)$ be the titania nanotubes ($\forall m, n \in \mathbb{N}$) with $6n(m+1)$ vertices and $10mn+8n$ edges, then from its structure, the vertex and edge partitions of

the vertex set $V(\text{TiO}_2(m,n))$ and edge set $E(\text{TiO}_2(m,n))$ and their order and size are as follow.¹⁷

$$\begin{aligned} V_2 &= \{v \in V(\text{TiO}_2(m,n)) \mid d_v = 2\}, \\ |V_2| &= 2mn + 4n \\ V_3 &= \{v \in V(\text{TiO}_2(m,n)) \mid d_v = 3\}, \\ |V_3| &= 2mn \\ V_4 &= \{v \in V(\text{TiO}_2(m,n)) \mid d_v = 4\}, \\ |V_4| &= 2n \\ V_5 &= \{v \in V(\text{TiO}_2(m,n)) \mid d_v = 5\}, \\ |V_5| &= 2mn \end{aligned} \quad (9)$$

and

$$\begin{aligned} E_6 &= \{uv \in E(\text{TiO}_2(m,n)) \mid d_u + d_v = 6\}, \\ |E_6| &= 6n \\ E_8^* &= \{uv \in E(\text{TiO}_2(m,n)) \mid d_u \times d_v = 8\}, \\ |E_8^*| &= 6n \end{aligned}$$

$$\begin{aligned} E_7 &= \{uv \in E(\text{TiO}_2(m,n)) \mid d_u + d_v = 7\}, \\ |E_7| &= 4n(m+1) \end{aligned} \quad (10)$$

$$\begin{aligned} E_{10}^* &= \{uv \in E(\text{TiO}_2(m,n)) \mid d_u \times d_v = 10\}, \\ |E_{10}^*| &= 4mn + 2n \end{aligned}$$

$$\begin{aligned} E_{12}^* &= \{uv \in E(\text{TiO}_2(m,n)) \mid d_u \times d_v = 12\}, \\ |E_{12}^*| &= 2n \end{aligned}$$

$$\begin{aligned} E_8 &= E_{15}^* = \{uv \in E(\text{TiO}_2(m,n)) \mid d_u \times d_v = 8\}, \\ |E_8| &= |E_{15}^*| = 2n(3m-1) \end{aligned}$$

By above mentioned formulas, one can see that

$$\begin{aligned} |V(\text{TiO}_2(m,n))| &= (2mn + 4n) + 2mn + \\ &+ 2n + 2mn = 6n(m+1). \\ |E(\text{TiO}_2(m,n))| &= \frac{1}{2} [2 \times (2mn + 4n) + \\ &+ 3 \times 2mn + 4 \times 2n + 5 \times 2mn] = 10mn + 8n. \end{aligned} \quad (11)$$

Now, we have the following computations of the Randić, Sum-connectivity and Modify Randić Indices for the titania nanotubes $\text{TiO}_2(m,n) \forall m,n \in \mathbb{N}$.

$$\begin{aligned} R(\text{TiO}_2(m,n)) &= \sum_{uv \in E(\text{TiO}_2(m,n))} \frac{1}{\sqrt{d_u d_v}} \\ &= \sum_{uv \in E_6} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_{10}^*} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_{12}^*} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_{15}^*} \frac{1}{\sqrt{d_u d_v}} \\ &= (6n) \times \left(\frac{1}{\sqrt{2 \times 4}}\right) + 2n(2m+1) \times \left(\frac{1}{\sqrt{2 \times 5}}\right) + (2n) \times \left(\frac{1}{\sqrt{3 \times 4}}\right) + (6mn - 2n) \times \left(\frac{1}{\sqrt{3 \times 5}}\right) \\ &= 3n\sqrt{2} + \frac{n(2m+1)\sqrt{10}}{5} + \frac{\sqrt{3}}{3}n + \frac{\sqrt{15}}{15}(6mn - 2n) \\ &= \frac{2}{5}(\sqrt{15} + \sqrt{10})mn + \left(3\sqrt{2} + \frac{\sqrt{10}}{5} + \frac{\sqrt{3}}{3} + \frac{2\sqrt{15}}{15}\right)n. \end{aligned} \quad (12)$$

Thus the Randić connectivity index of $\text{TiO}_2(m,n)$ nanotubes is equal to

$$R(\text{TiO}_2(m,n)) = \left(\frac{2(\sqrt{15} + \sqrt{10})}{5}m + \left(\frac{45\sqrt{2} + 3\sqrt{10} + 5\sqrt{3} + 2\sqrt{15}}{15}\right)\right)n \quad (13)$$

Also,

$$\begin{aligned}
 X(TiO_2(m, n)) &= \sum_{uv \in E(TiO_2[m, n])} \frac{1}{\sqrt{d_u + d_v}} \\
 &= \sum_{uv \in E_6} \frac{1}{\sqrt{d_u + d_v}} + \sum_{uv \in E_7} \frac{1}{\sqrt{d_u + d_v}} + \sum_{uv \in E_8} \frac{1}{\sqrt{d_u + d_v}} \\
 &= \frac{6n}{\sqrt{2+4}} + \frac{4mn+2n}{\sqrt{2+5}} + \frac{2n}{\sqrt{3+4}} + \frac{6mn-2n}{\sqrt{3+5}} \\
 &= \sqrt{6}n + \frac{4n(m+1)\sqrt{7}}{7} + \frac{\sqrt{2}}{2}n(3m-1).
 \end{aligned} \quad (14)$$

Hence the Sum-Connectivity index of $TiO_2(m, n)$ nanotubes is

$$\begin{aligned}
 X(TiO_2(m, n)) &= \left(\left(\frac{3\sqrt{2}}{2} + \frac{4\sqrt{7}}{7} \right) m \right. \\
 &\quad \left. + \left(\sqrt{6} + \frac{4\sqrt{7}}{7} - \frac{\sqrt{2}}{2} \right) n \right).
 \end{aligned} \quad (15)$$

Now, by using Definition 1, we see that there are two modify edges partitions E_4^+ and E_5^+ for the titania nanotubes $TiO_2(m, n)$ ($\forall m, n \in \mathbb{N}$) as:

$$\begin{aligned}
 E_4^+ &= \{uv \in E(TiO_2(m, n)) \mid \text{Max}\{2, 4\} \\
 &= \text{Max}\{3, 4\} = 4\} = E_8^* \cup E_{12}^* \\
 |E_4^+| &= |E_8^*| + |E_{12}^*| = 6n + 2n = 8n
 \end{aligned} \quad (16)$$

$$\begin{aligned}
 E_5^+ &= \{uv \in E(TiO_2(m, n)) \mid \text{Max}\{2, 5\} : \\
 &= \text{Max}\{3, 5\} = 5\} = E_{10}^* \cup E_{15}^* \\
 |E_{15}^*| &= 4nm + 2n + 2n(3m-1) = 10mn.
 \end{aligned}$$

Therefore the Modify Randić index of $TiO_2(m, n)$ is equal to:

$$\begin{aligned}
 R'(TiO_2(m, n)) &= \sum_{uv \in E(TiO_2[m, n])} \frac{1}{\max\{d_u, d_v\}} \\
 &= \sum_{uv \in E_4^+} \frac{1}{\max\{d_u, d_v\}} + \sum_{uv \in E_5^+} \frac{1}{\max\{d_u, d_v\}} \\
 &= \frac{8n}{4} + \frac{10mn}{5} = 2mn + 2n = 2n(m+1).
 \end{aligned} \quad (17)$$

Here, we complete the proof of main theorem of this article and all main results are computed.

Corollary 2.1. Consider the titania nanotubes $TiO_2(m, n)$ $\forall m, n \in \mathbb{N}$ (Figure 1), with $6n(m+1)$ vertices and $10mn+8n$

edges. For enough large integer number m and n , the Randić, Sum-connectivity and Modify Randić Indices of $TiO_2(m, n)$ are equal to:

(1) The Randić Connectivity index

$$R(TiO_2^*[m, n]) \approx (2.814m + 5.9688)n.$$

(2) The Sum-Connectivity index

$$X(TiO_2^*[m, n]) \approx (3.6332m + 3.2542)n.$$

(3) The Modify Randić index

$$R(TiO_2(m, n)) = (2m + 2)n.$$

Corollary 2. 2. Consider $TiO_2(m, n)$ nanotubes, Corollary 1 implies that for enough large integer number $m, n \in \mathbb{N}$,

$$X(TiO_2(m, n)) > R(TiO_2(m, n)) > R'(TiO_2(m, n)).$$

3. Discussion

Now we study the change of the values of Randić, Sum-connectivity and Modify Randić Indices of $TiO_2(m, n)$ nanotubes when the parameters m and n are slightly changed. The graphs of these nanotubes corresponding to some small values of m and n are shown in Figure 2. Similarly, the values of the studied topological indices corresponding to small change in the values of m and n is summarized in Table 1.

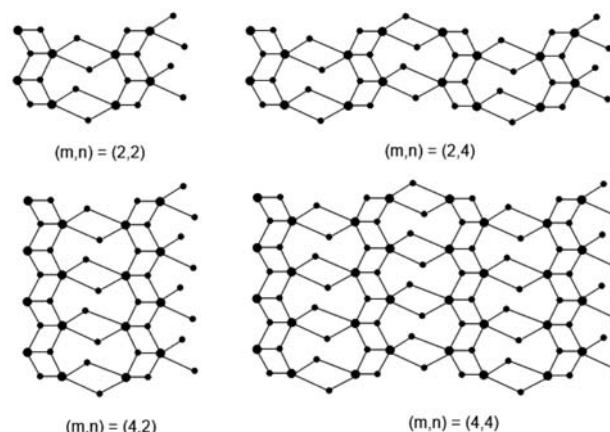


Figure 2. The graph of titania nanotubes $TiO_2(m, n)$ for $m = 2, 4$ and $n = 2, 4$.

4. Conclusion

In this paper, we considered an infinite class of the titania nanotubes $TiO_2(m, n)$, that were systematically

Table 1. Some values of Randić, Sum-connectivity and Modify Randić Indices of $TiO_2(m,n)$ nanotubes corresponding to the change in m and n .

	(m, n)	n = 1	n = 2	n = 3	n = 4
$R(G)$	m = 3	14.4112	28.8223	43.2335	57.6446
	m = 4	17.225	34.4505	51.6758	68.9010
$X(G)$	m = 3	14.1538	28.3076	42.4613	56.6151
	m = 4	17.7869	35.5739	53.3609	71.1478
$R'(G)$	m = 3	8	16	24	32
	m = 4	10	20	30	40

synthesized during the last 10–15 years using different methods and carefully studied as prospective technological materials. We computed its connectivity topological

indices including Randić index $R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-1/2}$,

Sum-Connectivity index $X(G) = \sum_{uv \in E(G)} (d_u + d_v)^{-1/2}$ and Mo-

lify Randić index $R'(G) = \sum_{uv \in E(G)} \frac{1}{\max\{d_u, d_v\}}$, that d_u and d_v are the degrees of the vertices u and v , respectively.

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Povzetek

Randićeve indeks povezanosti $R(G)$ je eden izmed najstarejših indeksov povezanosti, ki ga je uvedel Randić leta 1975. Drug indeks povezanosti je indeks vsote povezanosti $X(G)$, ki sta ga leta 2008 uvedla Zhou in Trinajstić. Nedavno, leta 2011 so Dvorak in sod. uvedli modificiran Randićev indeks povezanosti grafa G . V tem prispevku smo izračunali navedene topološke indekse povezanosti za družino molekulskih grafov znanih kot nanocevke $TiO_2(m,n)$.