THE RANDIĆ INDEX AND THE REDEFINED ZAGREB INDEX OF TITANIA NANOTUBES $TiO_2[m,n]$

Tomáš VETRÍK[1]

Values of the the Randić index and the redefined Zagreb indices for titania nanotubes $TiO_2[m,n]$ were presented in 2016 and 2017, but the values of the redefined second Zagreb index and the Randić index are incorrect. In this note we correct the mistakes and give exact values of these indices.

Keywords: Randić index, redefined Zagreb index, titania nanotube.

1. Introduction

A topological index is a numerical value associated with chemical constitution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. Let $V(G)$ be the vertex set and let $E(G)$ be the edge set of a simple connected graph G. Vertices correspond to the atoms of a compound and edges correspond to chemical bonds. The degree of a vertex $v \in V(G)$ is the number of neighbours of v, denoted by d_v. Chemical-based experiments indicate that there is strong relationship between the characteristics of chemical compounds and drugs and their molecular structures. Topological indices calculated for these chemical structures help us to understand the physical features, chemical reactivity and biological activity. A lot of research has been done on topological indices due to their chemical importance.

The Randić index

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

[1]Prof., Department of Mathematics and Applied Mathematics, University of the Free State, Bloemfontein, South Africa, e-mail: `vetrikt@ufs.ac.za`

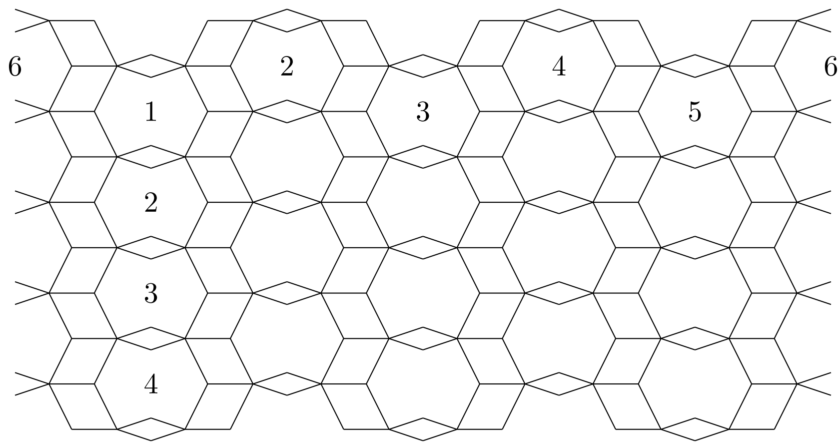

Fig. 1. Titania nanotube $TiO_2[m,n]$ for $m = 4$ and $n = 6$

of a graph G was introduced by the chemist Milan Randić in 1975, see [6]. This topological index has been successfully related to chemical and physical properties of organic molecules, and become one of the most important molecular descriptors. Graph-based molecular descriptors called the redefined Zagreb indices were introduced by Ranjini, Lokesha and Usha [7]. The redefined second Zagreb index of a graph G is defined as

$$ReZG_2(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}.$$

TiO_2 is one of the most studied compounds in materials science. Due to outstanding properties it is used for example in photocatalysis, biomedical devices and dye-sensitized solar cells. Bulk TiO_2 is a very useful environmentally friendly, non-toxic, corrosion-resistant material.

Values of the redefined first, second and third Zagreb indices for titania nanotubes $TiO_2[m,n]$ were presented by Gao et al. [4] and the values of the Randić index, the sum-connectivity index and the modified Randić index for titania nanotubes $TiO_2[m,n]$ were given by Gao, Farahani and Imran [3]. The values of the redefined second Zagreb index and the Randić index are incorrect. In this note we correct the mistakes and give exact values of these indices for titania nanotubes $TiO_2[m,n]$. Topological indices of nanotubes were investigated also in [1], [2] and [5].

2. **Results**

The two-dimensional lattice of the titania nanotube $TiO_2[m,n]$ for $m = 4$ and $n = 6$ is presented in Figure 1. Note that m is the number of hexagons in each column and n is the number of hexagons in each row. From Figure 1 it is easy to see that n must be even (and m is any positive integer). The number of vertices in this nanotube is equal to $(m+1)6n$ and the number of edges is

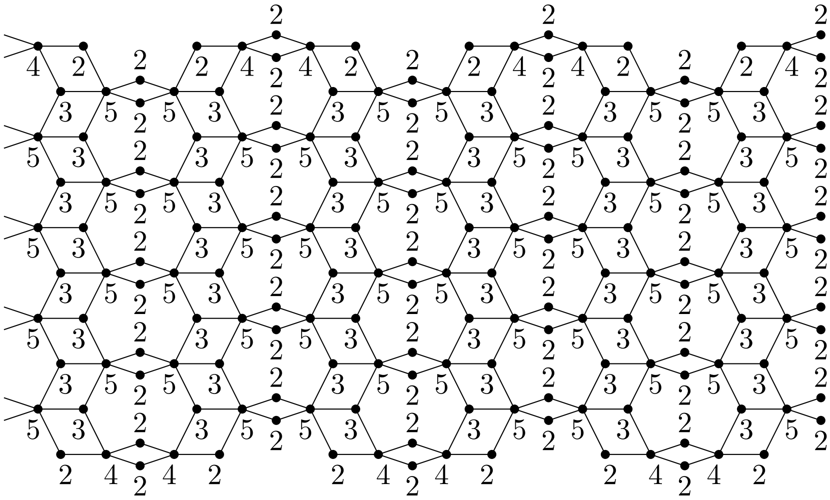

Fig. 2. Titania nanotube $TiO_2[4,6]$ with degrees assigned to the vertices

$(5m+4)2n$. We divide the vertices of G into four sets

$$V_i = \{v \in V(TiO_2[m,n]) \mid d_v = i\},$$

$i = 2,3,4,5$. So V_i contains the vertices of degree i. Note that $V(TiO_2[m,n]) = V_2 \cup V_3 \cup V_4 \cup V_5$. From Figure 2 we get

$$|V_2| = (m+2)2n,\ |V_3| = 2mn,\ |V_4| = 2n,\ |V_5| = 2mn.$$

Let

$$E_{i,j} = \{uv \in E(G) \mid d_u = i,\ d_v = j\}.$$

This means that the set $E_{i,j}$ contains the edges incident with one vertex of degree i and the other vertex of degree j. In Figure 2 we can see the degree of every vertex, thus we can easily get

$$|E_{5,3}| = (3m-1)2n,\ |E_{5,2}| = (2m+1)2n,\ |E_{4,3}| = 2n,\ |E_{4,2}| = 6n.$$

We have $E(TiO_2[m,n]) = E_{5,3} \cup E_{5,2} \cup E_{4,3} \cup E_{4,2}$. Let us use these sets to obtain the values of the Randić index for titania nanotubes $TiO_2[m,n]$.

Theorem 2.1. *The Randić index of titania nanotubes $TiO_2[m,n]$ is*

$$R(TiO_2[m,n]) = \frac{2(\sqrt{15}+\sqrt{10})mn}{5} + \Big(\frac{\sqrt{10}}{5} + \frac{\sqrt{3}}{3} + \frac{3\sqrt{2}}{2} - \frac{2\sqrt{15}}{15}\Big)n.$$

Proof. Since $E(TiO_2[m,n]) = E_{5,3} \cup E_{5,2} \cup E_{4,3} \cup E_{4,2}$, for the Randić index of titania nanotubes we have

$$\begin{aligned} R(TiO_2[m,n]) &= \sum_{uv \in E(TiO_2[m,n])} \frac{1}{\sqrt{d_u d_v}} \\ &= \sum_{uv \in E_{5,3}} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_{5,2}} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_{4,3}} \frac{1}{\sqrt{d_u d_v}} + \\ &\quad \sum_{uv \in E_{4,2}} \frac{1}{\sqrt{d_u d_v}} \\ &= \sum_{uv \in E_{5,3}} \frac{1}{\sqrt{5 \cdot 3}} + \sum_{uv \in E_{5,2}} \frac{1}{\sqrt{5 \cdot 2}} + \sum_{uv \in E_{4,3}} \frac{1}{\sqrt{4 \cdot 3}} + \\ &\quad \sum_{uv \in E_{4,2}} \frac{1}{\sqrt{4 \cdot 2}}. \end{aligned}$$

Let us note that $|E_{5,3}| = (3m-1)2n, |E_{5,2}| = (2m+1)2n, |E_{4,3}| = 2n$ and $|E_{4,2}| = 6n$, thus

$$\begin{aligned} R(TiO_2[m,n]) &= (3m-1)2n \cdot \frac{1}{\sqrt{15}} + (2m+1)2n \cdot \frac{1}{\sqrt{10}} + 2n \cdot \frac{1}{\sqrt{12}} + \\ &\quad 6n \cdot \frac{1}{\sqrt{8}} \\ &= \Big(\frac{3m-1}{\sqrt{15}} + \frac{2m+1}{\sqrt{10}} + \frac{1}{\sqrt{12}} + \frac{3}{\sqrt{8}}\Big)2n \\ &= \frac{2(\sqrt{15}+\sqrt{10})mn}{5} + \Big(\frac{\sqrt{10}}{5} + \frac{\sqrt{3}}{3} + \frac{3\sqrt{2}}{2} - \frac{2\sqrt{15}}{15}\Big)n. \end{aligned}$$

which is the exact value of the Randić index of titania nanotubes $TiO_2[m,n]$. □

Theorem 2.2. *The redefined second Zagreb index of titania nanotubes* $TiO_2[m,n]$ *is*

$$ReZG_2(TiO_2[m,n]) = \frac{(95m+59)5n}{28}.$$

Proof. Note that $E(TiO_2[m,n]) = E_{5,3} \cup E_{5,2} \cup E_{4,3} \cup E_{4,2}$, thus for the redefined second Zagreb index of titania nanotubes we have

$$\begin{aligned} ReZG_2(TiO_2[m,n]) &= \sum_{uv \in E(TiO_2[m,n])} \frac{d_u d_v}{d_u + d_v} \\ &= \sum_{uv \in E_{5,3}} \frac{5 \cdot 3}{5+3} + \sum_{uv \in E_{5,2}} \frac{5 \cdot 2}{5+2} + \sum_{uv \in E_{4,3}} \frac{4 \cdot 3}{4+3} + \\ &\quad \sum_{uv \in E_{4,2}} \frac{4 \cdot 2}{4+2}. \end{aligned}$$

Since $|E_{5,3}| = (3m-1)2n$, $|E_{5,2}| = (2m+1)2n$, $|E_{4,3}| = 2n$ and $|E_{4,2}| = 6n$, we obtain

$$\begin{aligned} E(TiO_2[m,n]) &= \Big((3m-1)\cdot\frac{15}{8} + (2m+1)\cdot\frac{10}{7} + \frac{12}{7} + 3\cdot\frac{4}{3}\Big)2n \\ &= \frac{(95m+59)5n}{28}, \end{aligned}$$

which is the value of the redefined second Zagreb index of titania nanotubes $TiO_2[m,n]$. □

3. Conclusion

In [4] at the bottom of page 275 the authors computed the redefined second Zagreb index of titania nanotubes $TiO_2[m,n]$ and they have

$$\frac{8}{6}(6n) + \frac{10}{7}(4mn+2n) + \frac{12}{7}(2n) + \frac{15}{8}(4mn-2n) = \frac{95n}{14}\Big(\frac{5m+2}{2}\Big)$$

which is incorrect, since we have

$$\frac{8}{6}(6n) + \frac{10}{7}(2n) + \frac{12}{7}(2n) - \frac{15}{8}(2n) = \frac{295n}{28}.$$

In [3] on page 258 the authors computed the Randić index of titania nanotubes $TiO_2[m,n]$ and there are two mistakes on this page. They have

$$(6n)\times\Big(\frac{1}{\sqrt{2\times 4}}\Big) = 3n\sqrt{2} \quad\text{and}\quad \frac{\sqrt{15}}{15}(6\text{mn}-2\text{n}) = \frac{2}{5}\sqrt{15}\text{mn} + \frac{2\sqrt{15}}{15}\text{n}.$$

They stated that the value of the Randić index of titania nanotubes $TiO_2[m,n]$ is about $(2.814m + 5.9688)n$. However, from our Theorem 2.1 it follows that the Randić index of these nanotubes is about $(2.814m+2.815)n$. By Theorem 2.1, the exact value of the Randić index of titania nanotubes $TiO_2[m,n]$ is

$$R(TiO_2[m,n]) = \frac{2(\sqrt{15}+\sqrt{10})mn}{5} + \Big(\frac{\sqrt{10}}{5} + \frac{\sqrt{3}}{3} + \frac{3\sqrt{2}}{2} - \frac{2\sqrt{15}}{15}\Big)n,$$

and by Theorem 2.2, the redefined second Zagreb index of titania nanotubes $TiO_2[m,n]$ is

$$ReZG_2(TiO_2[m,n]) = \frac{(95m+59)5n}{28}.$$

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