

# On the Second Harmonic Index of Titania Nanotubes

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Received: 📅 March 10, 2018; Published: 📅 March 19, 2018

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## Abstract

Topological indices which are graph invariants derived from molecular graphs of molecules are used in QSPR researches for modeling physicochemical properties of molecules. Topological indices are important tools for determining the underlying topology of a molecule in view of theoretical chemistry. The second harmonic index has been defined recently. In this study we compute the second harmonic index of Titania nanotubes.

**Keywords:** Harmonic Index; Novel Harmonic Indices; Second Harmonic Index; Titania Nanotube

## Introduction

Graph theory which is one of the most important branches of applied mathematics and chemistry has many applications from the basic sciences to the engineering sciences especially for solving and modeling of real world problems. Chemical graph theory is the common place for graph theory and chemistry. Topological indices are indispensable tools for QSPR researches in view of theoretical chemistry and chemical graph theory. Topological indices have been used more than seventy years predicting and modeling physicochemical properties of chemical substances. A graph  $G = (V, E)$  consists of two nonempty sets  $V$  and 2-element subsets of  $V$  namely  $E$ . The elements of  $V$  are called vertices and the elements of  $E$  are called edges. For a vertex  $v \in V$  show the number of edges that incident to  $v$ . The set of all vertices which adjacent to  $v$  is called the open neighborhood of  $v$  and denoted by  $N(v)$ . If we add the vertex  $v$  to  $N(v)$ , then we get the closed neighborhood of  $v$ ,  $N[v]$ . For the vertices  $u$  and  $v$ ,  $d(u, v)$  denotes the distance between  $u$  and  $v$  which means that minimum number of edges between  $u$  and  $v$ . The largest distance from the vertex  $v$  to any other vertex  $u$  called the eccentricity of  $v$  and denoted by  $e_v$ .

The first distance based topological index is the Wiener index which was defined by H. Wiener to modeling the boiling points of paraffin molecules [1]. In his study Wiener computed the all distances between the all atoms (vertices) in the molecular graph

of paraffin molecules and named this graph invariant as “path number”. The Wiener index of a simple connected graph  $G$  defined as follows:

$$W = W(G) = \sum_{\{u,v\} \in V(G)} d(u,v) \quad (1)$$

Many years later the path number renamed as “Wiener index” to honor Professor Harold Wiener for valuable contribution to mathematical chemistry. In the same year, the first degree based topological index was proposed by Platt for modeling physical properties of alkanes [2]. The Platt index of a simple connected graph  $G$  defined as follows;

$$I_{pl} = I_{pl}(G) = \sum_{uv \in E(G)} [\deg(u) + \deg(v) - 2] \quad (2)$$

After these both studies, approximately twenty five years later the well-known degree based Zagreb indices were defined by Gutman and Trinajstić to modeling  $\pi$ -electron energy of alternant carbons [3]. The first Zagreb index of a simple connected graph defined as;

$$M_1 = M_1(G) = \sum_{v \in V(G)} \deg(v)^2 \quad (3)$$

And the second Zagreb index of a simple connected graph defined as;

$$M_2 = M_2(G) = \sum_{uv \in E(G)} \deg(u)\deg(v) \quad (4)$$

An alternative definition of the second Zagreb index of a simple connected graph is given the following formula:

$$M_2 = M_2(G) = \sum_{uv \in E(G)} (\deg(u) + \deg(v)) \quad (5)$$

In 1975, Randić defined the "Randić index" [4] to modeling molecular branching of carbon skeleton atoms as follows:

$$R = R(G) = \sum_{uv \in E(G)} (\deg(u) \cdot \deg(v))^{-1/2} \quad (6)$$

Among the all topological indices, the above mentioned topological indices have been used for QSPR researches more considerably than any other topological indices in chemical and mathematical literature. We refer the interested reader to the following citations for up to date information about these well-known and the most used topological indices [5-15].

Harmonic index of a simple connected graph  $G$  was defined by Zhong in 2012 [16] as follows

$$H(G) = \sum_{uv \in E(G)} \frac{2}{\deg(u) + \deg(v)} \quad (7)$$

Since then, there are more than one hundred papers in mathematical and chemical literature about Harmonic index and its applications. We refer the interested reader to [17,18] and references cited in these articles.

The novel harmonic indices have been defined recently by the present authors [19]. In [19], the fifth harmonic index of H-Naphtalenic nanotube and TUC4 [m, n] nanotube were calculated.

Harmonic indices were defined in [20] as;

$$H_{general}(G) = \sum_{uv \in E(G)} \frac{2}{Q_u + Q_v} \quad (8)$$

Where  $Q_u$  is a unique parameter which is acquired from the vertex  $u \in (G)$ .

The first kind of this Harmonic indices was studied by Zhong by considering  $Q_u$  to be the degree of the vertex  $u$ :

$$H_1(G) = \sum_{uv \in E(G)} \frac{2}{\deg(u) + \deg(v)} \quad (9)$$

The second kind of this class was defined by considering  $Q_u$  to be the number  $n_u$  of vertices of  $G$  lying closer to the vertex  $u$  than to the vertex  $v$  for the edge  $uv$  of the graph  $G$ :

$$H_2(G) = \sum_{uv \in E(G)} \frac{2}{n_u + n_v} \quad (10)$$

The third type of this class was defined by considering  $Q_u$  to be the number  $m_u$  of edges of  $G$  lying closer to the vertex  $v$  than to the vertex  $u$  for the edge  $uv$  of the graph  $G$ :

$$H_3(G) = \sum_{uv \in E(G)} \frac{2}{m_u + m_v} \quad (11)$$

The fourth type of this class was defined by considering  $Q_u$  to be the eccentricity of the vertex  $u$ :

$$H_4(G) = \sum_{uv \in E(G)} \frac{2}{e_u + e_v} \quad (12)$$

The fifth type of this class was defined by considering  $Q_u$  to be the  $S_u = \sum_{v \in N(u)} \deg(v)$

$$H_5(G) = \sum_{uv \in E(G)} \frac{2}{S_u + S_v} \quad (13)$$

And the sixth type of this class was defined by considering  $Q_u$  to be the  $M_u = \prod_{v \in N(u)} \deg(v)$

$$H_6(G) = \sum_{uv \in E(G)} \frac{2}{M_u + M_v} \quad (14)$$

For topological indices of Titania nanotubes, we refer the interested reader [20-28] and references therein. The aim of this paper is to compute the exact value of the second harmonic index of Titania nanotubes.

## Results and Discussion

In this section we compute the exact values of the second harmonic index of Titania Nanotubes (Figure 1). Rezaei et al. [28] computed edge vertex version of Co-Pi index of Titania nanotubes [28]. The following table given the classifications of the vertices of  $TiO_2$  [m,n] with respect to the parameter  $n_u$ . We get the results with the help of the article of Rezaei et al. [30]. From the help of Table 1, we can state our main result (Figure 2).

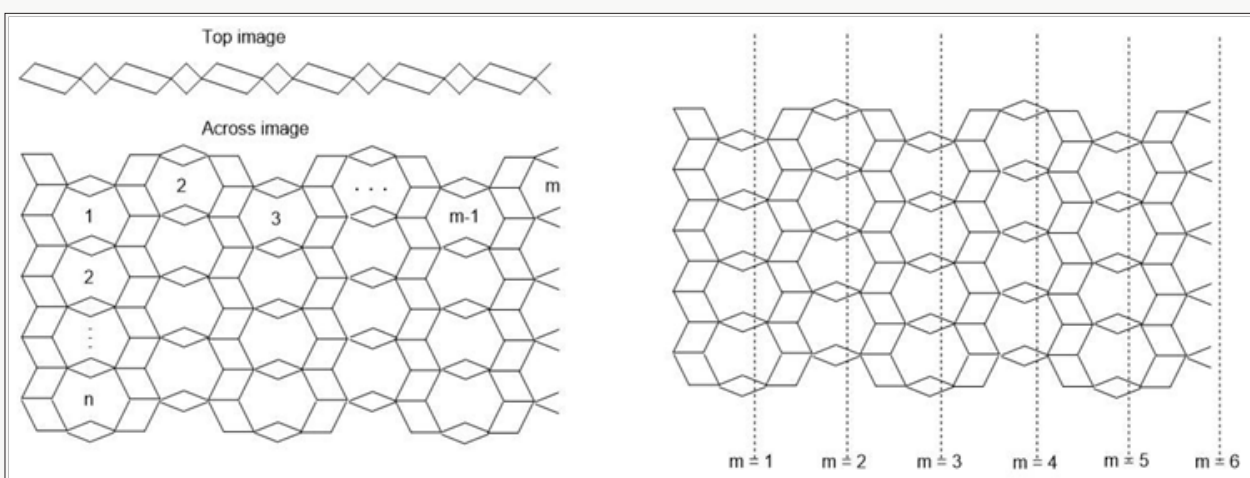
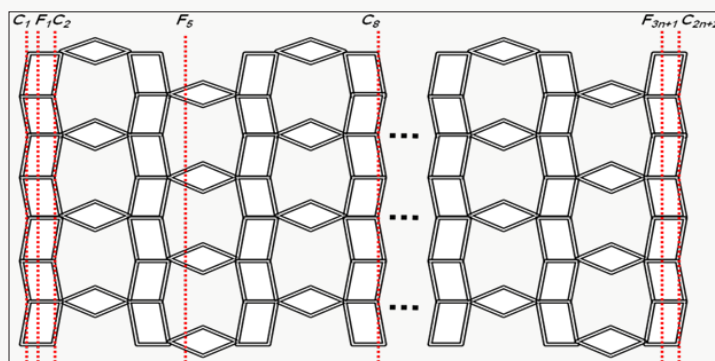


Figure 1: A graphical figure of Titania Nano tubes  $TiO_2$ [m, n].

**Table 1:** The edge classification of the vertices of TiO<sub>2</sub> [m, n] with respect to the parameter.

$n_v$ ; Edge: $e=uv$	The number of edge	$n_u$	$n_v$
$e_i = u_i v_i, i = 1, 2, \dots, n + 1$	$2(m + 1)$	$n_{u_i} = 2(m + 1)(3i - 2)$	$n_{v_i} = 2(m + 1)(3n - 3i + 4)$
$f_i = u_i v_i, i = 1, 2, \dots, n + 1$	$2m + 1$	$n_{u_i} = (m + 1)(6i - 5)$	$n_{v_i} = 3(m + 1)(2n - 2i + 3)$
$g_i = u_i v_i, i = 1, 2, \dots, n + 1$	$2m + 1$	$n_{u_i} = (m + 1)(6i + 3)$	$n_{v_i} = (m + 1)(6n - 6i + 1)$
$h_i = u_i v_i, i = 1, 2, \dots, n$	$2(m + 1)$	$n_{u_i} = 2(m + 1)(3i - 1)$	$n_{v_i} = 6(m + 1)(n - i + 1)$
$l_i = u_i v_i, i = 1, 2, \dots, n$	$2(m + 1)$	$n_{u_i} = 6i(m + 1)$	$n_{v_i} = 3(m + 1)(3n - 2i + 2)$

**Figure 2:** Orthogonal cuts representation of the Titania Nano tubes.

**Theorem 1.** The second harmonic index of Titania Nanotubes TiO<sub>2</sub>[m, n] is given as;

$$H_2(TiO_2[m, n]) = \frac{1}{3n+2} \left( \frac{2(2m+1)(n+1)}{m+1} + 4n + \frac{10}{3} \right)$$

**Proof.** From the definition of the second harmonic index and Table 1, we can write that:

$$\begin{aligned} H_2(TiO_2[m, n]) &= \sum_{uv \in E(TiO_2[m, n])} \frac{2}{n_u + n_v} \\ &= \sum_{uv \in e_i} \frac{2}{n_u + n_v} + \sum_{uv \in f_i} \frac{2}{n_u + n_v} + \sum_{uv \in g_i} \frac{2}{n_u + n_v} + \sum_{uv \in h_i} \frac{2}{n_u + n_v} + \sum_{uv \in l_i} \frac{2}{n_u + n_v} \\ &= \sum_{i=1}^{n+1} \frac{2(m+1)}{2(m+1)(3i-2) + 2(m+1)(3n-3i+4)} \\ &+ \sum_{i=1}^{n+1} \frac{2(m+1)}{(m+1)(6i-5) + 3(m+1)(2n-2i+3)} \\ &+ \sum_{i=1}^{n+1} \frac{2(m+1)}{(m+1)(6i+3) + (m+1)(6n-6i+1)} \\ &+ \sum_{i=1}^n \frac{2(m+1)}{2(m+1)(3i-1) + 6(m+1)(n-i+1)} \\ &+ \sum_{i=1}^n \frac{2(m+1)}{6i(m+1) + 3(m+1)(3n-2i+2)} \\ &= \frac{2(n+1)}{3n+2} + \frac{(n+1)2m+1}{3n+2} + \frac{(n+1)2m+1}{3n+2} + \frac{2n}{3n+2} + \frac{4}{3(3n+2)} \\ &= \frac{1}{3n+2} (2n+2 + \frac{2m+1}{m+1} (n+1) + \frac{2m+1}{m+1} (n+1) + 2n + \frac{4}{3}) \\ &= \frac{1}{3n+2} \left( \frac{2(2m+1)(n+1)}{m+1} + 4n + \frac{10}{3} \right) \end{aligned}$$

## Conclusion

In this study we found the exact values of newly defined the second harmonic index of Titania nanotube. This calculation will help to predict and model some physicochemical, optical and biological properties of Titania nanotube. It can be interesting to compute the novel harmonic topological indices of some other nanotubes and networks for further studies. It can also be interesting to study the mathematical and QSPR properties of these novel harmonic indices.

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DOI: [10.32474/DDIPIJ.2018.01.000102](https://doi.org/10.32474/DDIPIJ.2018.01.000102)



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