

Short communication

On Multiple Zagreb Indices of TiO_2 Nanotubes

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Abstract

The first and second Zagreb indices were first introduced by I. Gutman and N. Trinajstić in 1972. It is reported that these indices are useful in the study of anti-inflammatory activities of certain chemical instances, and in elsewhere. Recently, the first and second multiple Zagreb indices of a graph G were introduced by Ghorbani and Azimi in 2012. In this paper, we calculate the Zagreb indices and the multiplicative versions of the Zagreb indices of an infinite class of titania nanotubes $\text{TiO}_2[m,n]$.

Keywords: TiO_2 nanotubes, Topological indices, Zagreb index, Multiple Zagreb index

1. Introduction

Mathematical chemistry is a branch of theoretical chemistry in which we discuss and predict the chemical structure by using mathematical tools. Chemical graph theory is a branch of mathematical chemistry in which we apply tools from graph theory to model the chemical phenomenon mathematically. This theory plays a prominent role in the fields of chemical sciences.

A molecular graph is a simple graph in which the vertices denote atoms and the edges represent chemical bonds between these atoms. The hydrogen atoms are often omitted in a molecular graph. Let G be a molecular graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. We denote the order and size of G by $|V(G)|$ and $|E(G)|$, respectively. 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. The set of all vertices adjacent to a vertex u is said to be the neighbourhood of u , denoted as $N(u)$. The number of vertices in $N(u)$ is said to be the degree of u , denoted by $d(u)$. The maximum and minimum vertex degrees in a graph G , respectively denoted by $\Delta(G)$ and $\delta(G)$, are defined as $\max \{d(u) | u \in V(G)\}$ and $\min \{d(u) | u \in V(G)\}$, respectively. A (v_1, v_n) -path on n vertices is denoted by P_n and is defined as a graph with vertex set $\{v_i : 1 \leq i \leq n\}$ and edge set $v_i v_{i+1}$, for $1 \leq i \leq n-1$. The length of a path P_n is the number of edges in it, that is, $n-1$.

A topological index is a molecular graph invariant which correlates the physico-chemical properties of a

molecular graph with a number.¹ The first topological index was introduced by a chemist Harold Wiener in 1947 to calculate the boiling points of paraffins.² This numerical representation of a molecular graph has shown to be very useful quantity to use in the quantitative structure-property relationship.³ It also has many applications in communication, facility location, cryptography, etc., that are effectively modeled by a connected graph G with some restrictions.⁴ This index was originally defined for trees to correlate certain physico-chemical properties of alkanes, alcohols, amines and their compounds. Hosoya⁵ defined the notion of Wiener index for any graph G as

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

A pair of molecular descriptors known as the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ were first appeared in the topological formula for total π -energy of conjugated molecules that was derived in 1972 by Gutman and Trinajstić.⁶ Afterwards, these indices have been used as branching indices⁷. Later on, the Zagreb indices found applications in QSPR and QSAR studies.^{8,9} Many topological indices have been studied in the literature for different chemical structures.^{10–13}

The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a molecular graph G are respectively defined as

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 = \sum_{uv \in E(G)} (d(u) + d(v)) \quad (2)$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v). \quad (3)$$

The new multiplicative versions of $M_1(G)$ and $M_2(G)$ indices, denoted by $PM_1(G)$ and $PM_2(G)$ (respectively), were first defined by Ghorbani and Azimi.¹⁴ These indices are defined as follows.

$$PM_1(G) = \prod_{uv \in E(G)} (d_u + d_v), \quad (4)$$

$$PM_2(G) = \prod_{uv \in E(G)} d(u)d(v). \quad (5)$$

In this paper, we study the Zagreb and multiplicative versions of Zagreb indices of titania TiO_2 nanotubes. As a well-known semiconductor with numerous technological applications, Titania nanotubes are comprehensively studied in materials science. 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.¹⁵

Recently, the multiple Zagreb indices of circumcoronene homologous series of benzenoids were studied by Farahani.¹⁶ The Zagreb indices of some other nanotubes and benzenoid graphs can also be found in the literature.^{17,18}

2. Main Results

The graph of the titania nanotube $TiO_2 [m, n]$ is presented in Figure 1, where m denotes the number of octa-

gons in a column and n denotes the number of octagons in a row of the Titania nanotube.

In the following, we perform some necessary calculations for computing the Zagreb indices and multiplicative versions of Zagreb indices defined in the previous section.

Let us define the partitions for the vertex set and edge set of the titania nanotube TiO_2 , for $\delta(G) \leq k \leq \Delta(G)$, $2\delta(G) \leq i \leq 2\Delta(G)$, and $\delta(G)^2 \leq j \leq \Delta(G)^2$, then we have

$$V_k = \{v \in V(G) | d(v) = k\}, \quad (6)$$

$$E_i = \{e = uv \in E(G) | d(u) + d(v) = i\}, \quad (7)$$

$$E_j^* = \{e = uv \in E(G) | d(u)d(v) = j\}. \quad (8)$$

In the molecular graph of TiO_2 nanotubes, we can see that $2 \leq d(v) \leq 5$. So, we have the vertex partitions as follows.

$$V_2 = \{u \in V(G) | d(u) = 2\}, \quad (9)$$

$$V_3 = \{u \in V(G) | d(u) = 3\}, \quad (10)$$

$$V_4 = \{u \in V(G) | d(u) = 4\}, \quad (11)$$

$$V_5 = \{u \in V(G) | d(u) = 5\}. \quad (12)$$

Similarly, the edge partitions of the graph of TiO_2 nanotubes are as follows.

$$E_6 = E_8^* = \{e = uv \in E(G) | d(u) = 2 \ \& \ d(v) = 4\}, \quad (13)$$

$$E_7 = E_{10}^* \cup E_{12}^* = \{e = uv \in E(G) | d(u) = 2 \ \& \ d(v) = 5\} \quad (14)$$

$$\cup \{e = uv \in E(G) | d(u) = 3 \ \& \ d(v) = 4\}, \quad (15)$$

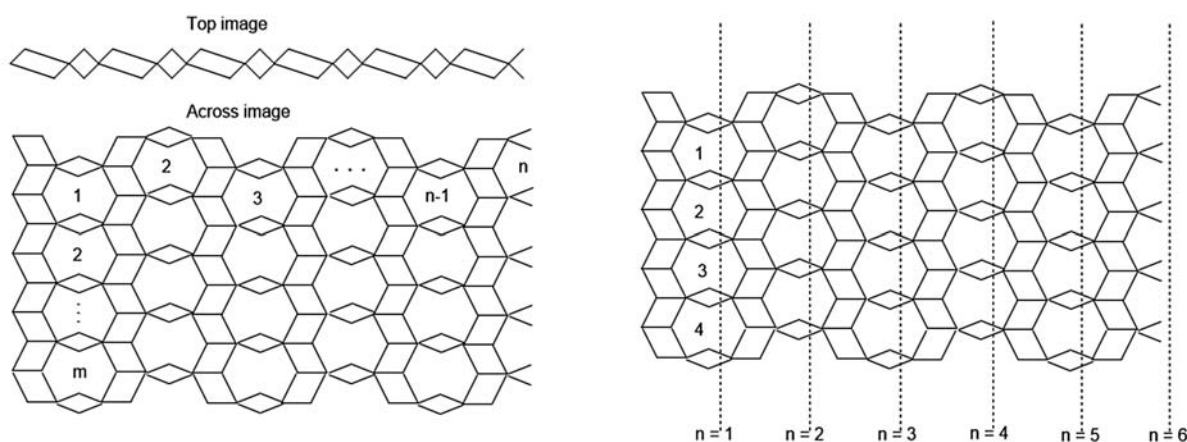


Figure 1: The graph of $TiO_2 [m, n]$ -nanotubes, for $m = 4$ and $m = 6$.

$$E_8 = E_{15}^* = \{e = uv \in E(G) \mid d(u) = 3 \text{ \& } d(v) = 5\}. \quad (16)$$

Since for every vertex $v \in V(G)$, $d(v)$ belongs to exactly one class V_k for $2 \leq k \leq 5$ and for every edge $uv \in E(G)$, $d(u) + d(v)$ (resp. $d(u)d(v)$) belongs to exactly one class E_i (resp. E_j^*) for $2\delta(G) \leq i \leq 2\Delta(G)$, and $\delta(G)^2 \leq j \leq \Delta(G)^2$. So, the vertex partitions V_k and the edge partitions E_i and E_j^* are collectively exhaustive, that is

$$\begin{aligned} \bigcup_{k=\delta(G)}^{\Delta(G)} V_k &= V(G), & \bigcup_{i=2\delta(G)}^{2\Delta(G)} E_i &= E(G), \\ \bigcup_{j=\delta^2(G)}^{\Delta^2(G)} E_j^* &= E(G). \end{aligned} \quad (17)$$

When $m = 1$, the number of vertices of degree 2 in $TiO_2[1, n]$ are $2n + n + 1 \times (2n) + n$. Thus for $TiO_2[m, n]$, we have $|V_2| = 2n + n + m(2n) + n = 2mn + 4n$. Similarly, the cardinalities of all the vertex and edge partitions can be obtained, which are presented in Table 1.

Table 1: The vertex and edge partitions of the TiO_2 nanotubes along with their cardinalities.

Vertex partition	Cardinality
V_2	$2mn + 4n$
V_3	$2mn$
V_4	$2n$
V_5	$2mn$
$E_6 = E_8^*$	$6n$
E_7	$4mn + 4n$
$E_8 = E_{15}^*$	$6mn - 2n$
E_{10}^*	$2mn + 2n$
E_{12}^*	$2n$

Theorem 2.1 The first Zagreb index of the TiO_2 nanotube is given by

$$M_1(TiO_2) = 76mn + 48n. \quad (18)$$

Proof. From equation 2, we have $M_1(TiO_2) = 6 \times |E_6| + 7 \times |E_7| + 8 \times |E_8|$. Using cardinalities of the edge partitions from Table 1, we get $M_1(TiO_2) = 76mn + 48n$, as required.

Theorem 2.2 The second Zagreb index of the TiO_2 nanotube is given by

$$M_2(TiO_2) = 130mn + 62n. \quad (19)$$

Proof. Using equation 3, we get $M_2(TiO_2) = 8 \times |E_8^*| + 10 \times |E_{10}^*| + 12 \times |E_{12}^*| + 15 \times |E_{15}^*|$. By cardinalities of the edge partitions from Table 1, we get $M_2(TiO_2) = 130mn + 62n$, as required.

Theorem 2.3 The first multiple Zagreb index of the TiO_2 nanotube is given by

$$PM_1(TiO_2) = 677376m^2n^4 + 112896mn^4 - 112896n^4. \quad (20)$$

Proof. From equation 4, we have $PM_1(TiO_2) = 6 \times |E_6| \times 7 \times |E_7| \times 8 \times |E_8|$. Using cardinalities of the edge partitions given in Table 1, we get $PM_1(TiO_2) = 677376m^2n^4 + 112896mn^4 - 112896n^4$, as required.

Theorem 2.4 The second multiple Zagreb index of the (TiO_2) nanotube is given by

$$PM_2(TiO_2) = 4147200m^2n^4 + 691200mn^4 - 691200n^4. \quad (21)$$

Proof. Using equation 5, we have $M_2(TiO_2) = 8 \times |E_8^*| \times 10 \times |E_{10}^*| \times 12 \times |E_{12}^*| \times 15 \times |E_{15}^*|$. By using cardinalities of the edge partitions from Table 1, we get $PM_2(TiO_2) = 4147200m^2n^4 + 691200mn^4 - 691200n^4$, as required.

3. Conclusion

The Zagreb indices were first appeared in the topological formula for the total π -energy of conjugated molecules that has been derived in 1972 by Gutman and Trinajstić³. These indices have also been used as branching indices and have found applications in QSPR and QSAR studies. In this paper, we studied the Zagreb indices and the newly defined multiplicative versions of the Zagreb indices of an infinite class of Titania nanotubes $TiO_2[m, n]$. Closed form formulas have been derived for the above mentioned indices.

4. References

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Povzetek

Prvi in drugi zagrebški indeks sta vpeljala I. Gutman in N. Trinajstić leta 1972. Izkazalo se je, da sta ta dva indeksa uporabna pri napovedih protivnetnih lastnosti nekaterih kemijskih spojin in drugih raziskavah. Ghorbani in Azimi sta prvi in drugi zagrebški indeks leta 2012 uporabila v grafu G. V tem delu smo zagrebška indeksa in njune večkratnike izračunali za nanocevke $TiO_2[m,n]$.