



Research Article

COMPUTING HYPER ZAGREB INDEX AND M-POLYNOMIALS OF  
TITANIA NANOTUBES  $TiO_2[m, n]$

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ABSTRACT

The concept of hyper Zagreb index, Zagreb and M-polynomials are establish in chemical graph theory based on the degree of the vertex. It is reported that these indices are useful in the study of anti-inflammatory activities of certain chemical networks. In this paper, we determine hyper Zagreb index, Zagreb and M-polynomials for an infinite class of Titania nanotubes  $TiO_2[m, n]$ .

**Keywords:** Hyper Zagreb index, Zagreb polynomials, M-polynomial,  $TiO_2$  nanotubes.

1. INTRODUCTION

In the last decade, graph theory has been found a considerable use in this area of research. Graph theory has provided chemist with a variety of useful tools, such as topological indices. Chem-informatics is new subject which is a combination of chemistry, mathematics and information science. It studies Quantitative structure-activity (QSAR) and structure-property (QSPR) relationships that are used to predict the biological activities and properties of chemical compounds. In the QSAR /QSPR study, physico-chemical properties and topological indices such as hyper Zagreb index, first multiple Zagreb index, second multiple Zagreb index and Zagreb polynomials are used to predict bioactivity of the chemical compounds.

More preciously 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.

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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  $V(G) = \{a_1, a_2, \dots, a_n\}$  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  $a$  and  $b$  is denoted by  $ab$ . Two vertices  $a$  and  $b$  are said to be adjacent if there is an edge between them. The set of all vertices adjacent to a vertex  $a$  is said to be the neighbourhood of  $a$ , denoted as  $N(a)$ . The number of vertices in  $N(a)$  is said to be the degree of  $a$ , denoted by  $d(a)$ . The maximum and minimum vertex degrees in a graph  $G$ , respectively denoted by  $\Delta(G)$  and  $\delta(G)$ , are defined as  $\max\{d(a) \mid a \in V(G)\}$  and  $\min\{d(a) \mid a \in V(G)\}$ , respectively. A  $(a_1, a_n)$ -path on  $n$  vertices is denoted by  $P_n$  and is defined as a graph with vertex set  $\{a_i : 1 \leq i \leq n\}$  and edge set  $a_i a_{i+1}$ , 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 numeric quantity associated with a graph which characterizes the topology of graph and is invariant under graph automorphism. There are some major classes of topological indices such as distance based topological indices, degree based topological indices and counting related polynomials and indices of graphs. Among these classes degree based topological indices are of great importance and play a vital role in chemical graph theory and particularly in chemistry. In more precise way, a topological index  $Top(G)$  of a graph  $G$ , is a number with the property that for every graph  $H$  isomorphic to  $G$ ,  $Top(H) = Top(G)$ . The concept of topological index came from work done by Wiener [1], while he was working on boiling point of paraffin. He named this index as path number. Later on, the path number was renamed as Wiener index. The Wiener index is the first and most studied topological index, both from theoretical point of view and applications, and defined as the sum of distances between all pairs of vertices in  $G$ , see for details [2].

One of the oldest topological index is the first and second Zagreb index an introduced by I. Gutman and N. Trinajstić [3] on based degree of vertices of  $G$  in 1972 and are defined as:

$$M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)], \quad M_2(G) = \sum_{uv \in E(G)} [d(u) \times d(v)]$$

M. Ghorbani and N. Azimi [4] define two new versions of Zagreb indices of a graph  $G$  in 2012. The first multiple Zagreb index  $PM_1(G)$ , second multiple Zagreb index  $PM_2(G)$  and these indices are defined as:

$$PM_1(G) = \prod_{uv \in E(G)} [d(u) + d(v)], \quad PM_2(G) = \prod_{uv \in E(G)} [d(u) \times d(v)]$$

In 2013, G.H. Shirdel, H. RezaPour and A.M. Sayadi [5] introduced a new degree based of Zagreb index named 'hyper Zagreb index' as

$$HM(G) = \sum_{uv \in E(G)} [d(u) + d(v)]^2 \tag{1}$$

In 2004, I. Gutman and K.C. Das [6] define the first and second Zagreb Polynomial in the following way.:

$$M_1(G, x) = \sum_{uv \in E(G)} x^{[d(u)+d(v)]} \tag{2}$$

$$M_2(G, x) = \sum_{uv \in E(G)} x^{[d(u) \times d(v)]} \tag{3}$$

The properties of  $M_1(G, x)$ ,  $M_2(G, x)$  polynomials for some chemical structures have been studied in the literature [6-10].

In 2015, E. Deutshi and S. Klavžar [11] define a new polynomial namely ‘M-polynomial’ based on the degree of the vertex in the following way:

$$M_1(G, x, y) = \sum_{uv \in E(G)} x^{[d(u)]} y^{[d(v)]} \tag{4}$$

Motivated by the idea of E. Deutshi and S. Klavžar [11], we define the multiplicative version of ‘M- polynomial’ in the following way.

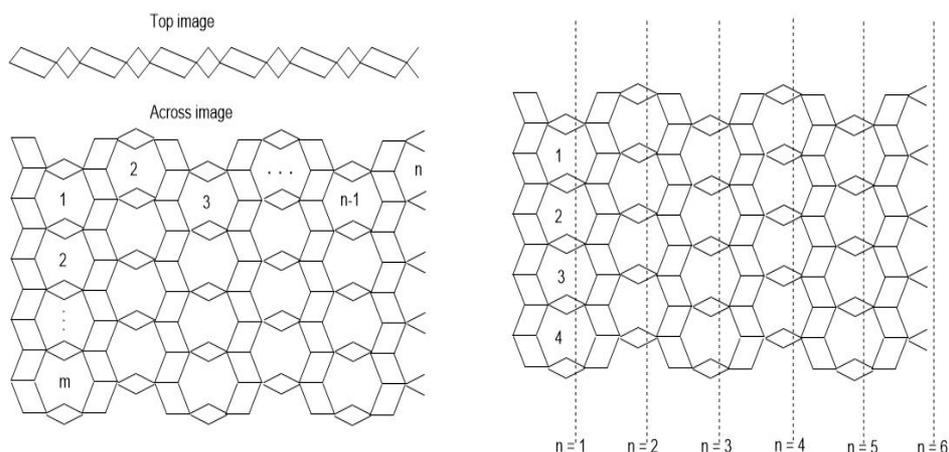
$$M_2(G, x, y) = \prod_{w \in E(G)} x^{[d(u)]} y^{[d(v)]} \tag{5}$$

Nowadays there is an extensive research activity on  $HM(G)$ ,  $PM_1(G)$ ,  $M_2(G)$  indices and  $M_1(G, x)$ ,  $M_1(G, x)$ ,  $M(G, xy)$ ,  $M_1(G, x, y)$  and their variants, For further study of topological indices of various graph families, see [12-20].

## 2. TITANIA NANOTUBE $TiO_2[m, n]$

Titania nanotubes comprehensively study 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 [21-36].

The graph of the Titania nanotube  $TiO_2[m, n]$  is presented in Figure 1, where  $m$  denotes the number of octagons in a column and  $n$  denotes the number of octagons in a row of the Titania nanotube.



**Figure 1.** For  $m = 4$  and  $n = 6$ , the graph of  $TiO_2[m, n]$ -nanotubes

M.A. Malik and M. Imran [37] compute the first and second Zagreb index, first and second multiple Zagreb index for an infinite class of Titania nanotubes  $TiO_2[m, n]$ . In the next Theorems we compute hyper Zagreb index, Zagreb and M- polynomials for an infinite class of Titania nanotubes  $TiO_2[m, n]$ .

For this we perform some necessary calculations for computing the hyper Zagreb index, Zagreb and M-polynomials 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

$$\begin{aligned} V_k &= \{v \in V(G) \mid d(v) = k\}, \\ E_i &= \{e = uv \in E(G) \mid d(u) + d(v) = i\}, \\ E_j^* &= \{e = uv \in E(G) \mid d(u)d(v) = j\}. \end{aligned}$$

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.

$$\begin{aligned} V_2 &= \{u \in V(G) \mid d(u) = 2\}, \\ V_3 &= \{u \in V(G) \mid d(u) = 3\}, \\ V_4 &= \{u \in V(G) \mid d(u) = 4\}, \\ V_5 &= \{u \in V(G) \mid d(u) = 5\}. \end{aligned}$$

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

$$\begin{aligned} E_6 &= E_8^* = \{e = uv \in E(G) \mid d(u) = 2 \ \& \ d(v) = 4\}, \\ E_7 &= E_{10}^* \cup E_{12}^* = \{e = uv \in E(G) \mid d(u) = 2 \ \& \ d(v) = 5\} \\ &\cup \{e = uv \in E(G) \mid d(u) = 3 \ \& \ d(v) = 4\}, \\ E_8 &= E_{15}^* = \{e = uv \in E(G) \mid d(u) = 3 \ \& \ d(v) = 5\}. \end{aligned}$$

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

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

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 partitions of the  $TiO_2$  nanotubes along with their cardinalities.

<b>Vertex partition</b>	$V_2$	$V_3$	$V_4$	$V_5$
<b>Cardinality</b>	$2mn+4n$	$2mn$	$2n$	$2mn$

**Table 2.** The edge partitions of the  $TiO_2$  nanotubes along with their cardinalities.

<b>Vertex partition</b>	$E_6 = E_8^*$	$E_7$	$E_8 = E_{15}^*$	$E_{10}^*$	$E_{12}^*$
<b>Cardinality</b>	$6n$	$4mn+4n$	$6mn-2n$	$4mn+2n$	$2n$

Now we compute hyper Zagreb index, Zagreb polynomials and M-polynomials in the following theorems.

**Theorem 1.** The hyper Zagreb index of the  $TiO_2$  nanotube is given by

$$HM(TiO_2) = 284n + 580mn.$$

*Proof.* From equation (1) and using cardinalities of the edge partitions from Table 2, we get,

$$\begin{aligned} HM(TiO_2) &= \sum_{uv \in E(G)} [d(u) + d(v)]^2 \\ &= \sum_{uv \in E_6(TiO_2)} [d(u) + d(v)]^2 + \sum_{uv \in E_7(TiO_2)} [d(u) + d(v)]^2 + \sum_{uv \in E_8(TiO_2)} [d(u) + d(v)]^2 \\ &= 36(|E_6(TiO_2)|) + 49(|E_7(TiO_2)|) + 64(|E_8(TiO_2)|) \\ &= 36(6n) + 49(4mn + 4n) + 64(6mn - 2n) \\ &= 284n + 580mn. \end{aligned}$$

**Theorem 2.** The first Zagreb polynomial of the  $TiO_2$  nanotube is given by

$$M_1(TiO_2, x) = (6n)x^6 + (4mn + 4n)x^7 + (6mn - 2n)x^8.$$

*Proof.* From equation (2) and using cardinalities of the edge partitions from Table 2, we get,

$$\begin{aligned} M_1(TiO_2, x) &= \sum_{uv \in E(TiO_2)} x^{[d(u)+d(v)]} \\ &= \sum_{uv \in E_6(TiO_2)} x^{[d(u)+d(v)]} + \sum_{uv \in E_7(TiO_2)} x^{[d(u)+d(v)]} + \sum_{uv \in E_8(TiO_2)} x^{[d(u)+d(v)]} \\ &= (|E_6(TiO_2)|)x^6 + (|E_7(TiO_2)|)x^7 + (|E_8(TiO_2)|)x^8 \\ &= (6n)x^6 + (4mn + 4n)x^7 + (6mn - 2n)x^8. \end{aligned}$$

**Theorem 3.** The second Zagreb polynomial of the  $TiO_2$  nanotube is given by

$$M_2(TiO_2, x) = (6n)x^8 + (4mn + 4n)x^{10} + (6mn - 2n)x^{15}.$$

*Proof.* From equation (3) and using cardinalities of the edge partitions from Table 2, we get,

$$\begin{aligned}
 M_2(TiO_2, x) &= \sum_{uv \in E(TiO_2)} x^{[d(u) \times d(v)]} \\
 &= \sum_{uv \in E_6(TiO_2)} x^{[d(u) \times d(v)]} + \sum_{uv \in E_7(TiO_2)} x^{[d(u) \times d(v)]} + \sum_{uv \in E_8(TiO_2)} x^{[d(u) \times d(v)]} \\
 &= (|E_6(TiO_2)|)x^8 + (|E_7(TiO_2)|)x^{10} + (|E_8(TiO_2)|)x^{15} \\
 &= (6n)x^8 + (4mn + 4n)x^{10} + (6mn - 2n)x^{15}.
 \end{aligned}$$

**Theorem 4.** The first M- polynomial of the  $TiO_2$  nanotube is given by

$$M_1(TiO_2, x, y) = (6n)x^2y^4 + (4mn + 4n)x^2y^5 + (6mn - 2n)x^3y^5.$$

*Proof.* From equation (4) and using cardinalities of the edge partitions from Table 2, we get,

$$\begin{aligned}
 M_1(TiO_2, x, y) &= \sum_{uv \in E(TiO_2)} x^{[d(u)]}y^{[d(v)]} \\
 &= \sum_{uv \in E_6(TiO_2)} x^{[d(u)]}y^{[d(v)]} + \sum_{uv \in E_7(TiO_2)} x^{[d(u)]}y^{[d(v)]} + \sum_{uv \in E_8(TiO_2)} x^{[d(u)]}y^{[d(v)]} \\
 &= (|E_6(TiO_2)|)x^2y^4 + (|E_7(TiO_2)|)x^2y^5 + (|E_8(TiO_2)|)x^3y^5 \\
 &= (6n)x^2y^4 + (4mn + 4n)x^2y^5 + (6mn - 2n)x^3y^5.
 \end{aligned}$$

**Theorem 5.** The second M- polynomial of the  $TiO_2$  nanotube is given by

$$M_2(TiO_2, x, y) = x^{26mn+16n}y^{50mn+32n}$$

*Proof.* From equation (5) and using cardinalities of the edge partitions from Table 2, we get,

$$\begin{aligned}
 M_2(TiO_2, x, y) &= \prod_{uv \in E(TiO_2)} x^{[d(u)]}y^{[d(v)]} \\
 &= \prod_{uv \in E_8^*(TiO_2)} x^{d(u)}y^{d(v)} \times \prod_{uv \in E_{10}^*(TiO_2)} x^{d(u)}y^{d(v)} \times \prod_{uv \in E_{12}^*(TiO_2)} x^{d(u)}y^{d(v)} \times \prod_{uv \in E_{15}^*(TiO_2)} x^{d(u)}y^{d(v)} \\
 &= (x^2y^4)^{|E_8^*(TiO_2)|} \times (x^2y^5)^{|E_{10}^*(TiO_2)|} \times (x^3y^4)^{|E_{12}^*(TiO_2)|} \times (x^3y^5)^{|E_{15}^*(TiO_2)|} \\
 &= (x^2y^4)^{(6n)} \times (x^2y^5)^{(4mn+2n)} \times (x^3y^4)^{(2n)} \times (x^3y^5)^{(6mn-2n)} \\
 &= (x^{12n}y^{24n})(x^{2(4mn+2n)}y^{5(4mn+2n)})(x^{6n}y^{8n})(x^{3(6mn-2n)}y^{5(6mn-2n)}) \\
 &= x^{26mn+16n}y^{50mn+32n}.
 \end{aligned}$$

### 3. CONCLUSION

Since Topological indices have also been used as branching indices and have found applications in QSPR and QSAR studies. In this paper, we have deal with Titania nanotubes and studied their topological indices. More preciously, we determine hyper Zagreb index, Zagreb and M-polynomials for an infinite class of Titania nanotubes  $TiO_2[m, n]$ . In the future, we are interested to design some new architectures/networks and then study their topological indices which will be quite helpful to understand their underlying topologies.

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