# ON ZAGREB INDICES AND ZAGREB POLYNOMIALS OF SINGLE-WALLED TITANIA NANOTUBES

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***ABSTRACT**: The degree of a vertex of a molecular graph is the number of first neighbors of this vertex. A large number of molecular-graph-based structure descriptors (topological indices) have been conceived, depending on vertex degrees. Topological indices are numerical values of a graph which characterize its topology and are usually graph invariants. Realizing the significance of these graph invariants, in this paper, we compute and provide closed formulae of Zagreb indices, multiple Zagreb indices and Zagreb Polynomials for single-walled titania nanotubes.*

**Keywords:** $TiO_2$ nanotubes; Topological indices; Zagreb index; Augmented Zagreb index; Zagreb polynomials.

## INTRODUCTION

The branch of chemistry in which we discuss and predict the chemical structure by using mathematical tools without referring to quantum mechanics is called *mathematical chemistry* [1, 2]. The branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena is known as *chemical graph theory* [2]. This theory had a vital role in the development of the chemical sciences.

A *molecular graph* is a simple graph in which atoms are denoted by vertices and chemical bonds between these atoms are represented by edges. In a molecular graph, the hydrogen atoms are often omitted. Let $G$ be a molecular graph with vertex set $V(G)$ and edge set $E(G)$. We denote the *order* of $G$ by $|V(G)|$ and *size* of G by $|E(G)|$. An edge in $E(G)$ with end vertices $u$ and $v$ is denoted by $uv$. Two vertices $u$ and $v$ are called *adjacent* if there is an edge between them. The *neighborhood* of $u$, denoted by $N(u)$, is the set of all vertices adjacent to u. The *degree* of u is denoted by $d_u$ and equals $|N(u)|$.

Topological indices are the numerical values that correlate the chemical structure with various physical properties, chemical reactivity or biological activity. The topological index describes the structure and the branching pattern of the molecule numerically. Therefore, the topological analysis of a molecule assigns unique number (index) to the structure of the molecule, that may be considered a descriptor of the molecule under examination. The topological indices play a vital role in quantitative structure-activity research ($QSAR$) and structure-property relationships research ($QSPR$) study.

Titania is one of the most comprehensively studied metal oxide substances due to its wide spread applications in production of catalytic, gas-sensing and corrosion-resistance materials [3]. $TiO_2$ attracts considerable technological interest due to unique properties in biology, optics, electronics and photo-chemistry [4]. Recent experimental studies show that titania nanotubes $(NTs)$ improve $TiO_2$ bulk properties for photocatalysis, hydrogen-sensing and photo-voltaic applications [5]. Various titania nanotubes were observed in two types of morphologies: multi-walled $(MW)$ cylindrical and scroll-like frequently containing various types of defects and impurities [6].

Historically, the first vertex-degree-based structure descriptors were the graph invarients that now-a-days are called Zagreb indices [7, 8]. It is interesting that these were used for a completely different purpose and were included among topological indices much later. The terms, $\sum_{v\in V(G)} d_v^2$, $\sum_{uv\in E(G)} d_u d_v$ and $\sum_{v\in V(G)} d_v^3$ were first appeared in the topological formula for total $\pi$-energy of conjugated molecules that was derived in 1972 by Gutman and Trinajstiс′ [7]. Ten years later, Balaban et al. included

$$M_1(G) = \sum_{v\in V(G)} d_v^2 = \sum_{uv\in E(G)} (d_u + d_v) \qquad (1)$$

and

$$M_2(G) = \sum_{uv\in E(G)} d_u d_v \qquad (2)$$

among topological indices and named them " Zagreb group indices" [9]. The reason was that both the authors of [7] were members of the Theoretical Chemistry Group of the " Ruder Boškoviс′ " Institute in Zagreb. The name "Zagreb group indices" was abbreviated to " Zagreb indices " and now we call $M_1(G)$, the first Zagreb index and $M_2(G)$, the second Zagreb index. Afterward these indices have been used as branching indices [10]. Later on the Zagreb indices found applications in QSPR and QSAR studies [1, 11]. These indices have been used to study molecular complexity, chirality, $ZE$-isomorphism and hetero-systems. Their chemical applications and mathematical properties can be studied from [12, 13, 14, 15, 16, 17, 18, 19].

The term, $\sum_{v\in V(G)} (d_v)^3$ was ignored for the next more than forty years. Recently, Furtula and Gutman proved that this term have a very promising application potential [20]. They proposed that this term should be named the forgotten topological index or shortly the F-index that is defined as

$$F(G) = \sum_{v\in V(G)} (d_v)^3 = \sum_{uv\in E(G)} [(d_u)^2 + (d_v)^2]. \qquad (3)$$

They discovered a remarkable fact that the linear combination $M_1 + \lambda F$ yields a highly accurate mathematical model of certain physico-chemical properties of alkanes [20].

Another important graph invariant that is necessarily encountered within studies of the difference between the two

Zagreb indices [21], is the reduced second Zagreb index, defined as

$$RM_2(G) = \sum_{uv\in E(G)} (d_u - 1)\times(d_v - 1). \qquad (4)$$

The augmented Zagreb index of $G$ proposed by Furtula et al. in 2010 [22] is defined as

$$AZI(G) = \sum_{uv\in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3. \qquad (5)$$

This graph invariant has proven to be valuable predictive index in the study of the heat of formation in octanes and heptanes [22]. Noting that if instead of the exponent $3$ we would set $-0.5$, then we would arrive at the ordinary $ABC$ index. Preliminary studies [22, 15, 23] indicate that $AZI$ has an even better correlation potential than $ABC$ index. The third Zagreb index was introduced by Shirdel in 2013 [24], defined as

$$M_3(G) = \sum_{uv\in E(G)} (d_u + d_v)^2. \qquad (6)$$

Clearly, this index is a combination of F-index and the second Zagreb index i.e

$$M_3(G) = F(G) + 2M_2(G). \qquad (7)$$

Because of the above mentioned relation, we studied the F-index with the indices of the Zagreb family.

The degree product $P(G) = \prod_{v\in V(G)} d_v$ of a graph G was introduced and studied by Narumi and Katayama for the first time. The Narumi-Katayama index was proposed in 1984, by Narumi and Katayama [25]. It is defined as

$$NK(G) = \prod_{v\in V(G)} d_v. \qquad (8)$$

The first and second multiple Zagreb indices were introduced by Ghorbani and Azimi in 2012 [26], defined as

$$PM_1(G) = \prod_{uv\in V(G)} (d_u + d_v) = \prod_{v\in V(G)} (d_v)^2 \qquad (9)$$

and

$$PM_2(G) = \prod_{uv\in V(G)} (d_u d_v). \qquad (10)$$

Clearly, the first multiple Zagreb index is the square of Narumi-Katayama index. In 2009, Fath-Tabar [27] put forward the first and the second Zagreb polynomials of the graph $G$, defined respectively as

$$ZG_1(G,x) = \sum_{uv\in E(G)} x^{d_u + d_v} \qquad (11)$$

and

$$ZG_2(G,x) = \sum_{uv\in E(G)} x^{d_u d_v}, \qquad (12)$$

where $x$ is a dummy variable.

The first Zagreb index, the second Zagreb index, the first multiple Zagreb index and the second multiple Zagreb index have been computed for six-layered single-walled titania nanotube [28]. In this paper we study two types of titania nanotubes based on their structural layers in underlying chemical structure: three-layered single-walled titania nanotubes and six-layered single-walled titania nanotubes.

## ZAGREB INDICES AND ZAGREB POLYNOMIALS FOR THREE-LAYERED SINGLE-WALLED TITANIA NANOTUBE

Titania $NTs$ exist in nature in two forms namely, single-walled titania $(SW\,TiO_2)$ nanotubes and multi-walled titania $(MW\,TiO_2)$ nanotubes. Our study mainly focuses on the single-walled $TiO_2$ nanotubes because we consider their chemical graphs to work on molecular descriptors. Anatase is one of the three mineral forms of titanium dioxide, the other two being brookite and rutile [29]. Titania nanotubes are formed by rolling up the stoichiometric two-periodic $(2D)$ sheets cut from the energetically stable anatase surface, which contains either six $(O-Ti-O-O-Ti-O)$ or three $(O-Ti-O)$ layers [29]. We denote the 2-parametric chemical graph of three-layered titania nanotubes as $TNT_3[m,n]$, where $m$ and $n$ are number of titanium atoms in each column and row respectively. Which can be viewed in Figure 1.

The size of $TNT_3[m,n]$ is $12mn+2m$. There are four kinds of edges corresponding to their degrees of end vertices. The edge partition of edge set of $TNT_3[m,n]$ is shown in Table 1.

The order of $TNT_3[m,n]$ is $6mn+3m$. There are four kinds of vertices in the set $V(G)$ corresponding to their degrees. Table 2 shows such a partition of the set $V(G)$ of $TNT_3[m,n]$.

The following theorems present the analytically closed formulae of Zagreb indices and Zagreb polynomials for this nanotube.

**Theorem 1** The first and second Zagreb indices for $G = TNT_3[m,n]$ are given by

$M_1(G) = 6m(18n-1)$ and $M_2(G) = 4m(54n-13)$.

Proof. Using equation (1) and Table 1, we have

$$M_1(G) = \sum_{uv\in E(G)} (d_u + d_v)$$
$$= 4m(2+4) + 4m(3+4) + 4m(2+6) + 2m(6n-5)(3+6).$$

After simplification we get the required result, $M_1(G) = 6m(18n-1)$.

Similarly, Using equation (2) and Table 1, we have

$$M_2(G) = \sum_{uv\in E(G)} (d_u d_v)$$
$$= 4m(2)(4) + 4m(3)(4) + 4m(2)(6)$$
$$+ 2m(6n-5)(3)(6) = 4m(54n-13).$$

**Theorem 2** The reduced second Zagreb index for $G = TNT_3[m,n]$ is given by

$RM_2(G) = 4m(30n-11)$.

Proof. Using equation (4) and Table 1, we find

$$RM_2(G) = \sum_{uv\in E(G)} (d_u - 1)\times(d_v - 1)$$

$= 4m(3)+4m(6)+4m(5)+2m(6n-5)(10)$.

After simplification we get the required result, $RM_2(G) = 4m(30n-11)$.

**Theorem 3** The third Zagreb index for $G = TNT_3[m,n]$ is given by

$$M_3(G) = 2m(486n-107).$$

Proof. Using equation (6) and Table 1, we get

$$M_3(G) = \sum_{uv\in E(G)} (d_u + d_v)^2$$

$$= 4m(6)^2 + 4m(7)^2 + 4m(8)^2 + 2m(6n-5)(9)^2.$$

After simplification we get the required result, $M_3(G) = 2m(486n-107)$.

**Lemma 1** The F-index for $G = TNT_3[m,n]$ is given by

$$F(G) = 10m(54n-11).$$

Proof. Using equation (7), Theorem 1 and Theorem 3, we get

$$F(G) = 2m(486n-107) - 24m(54n-13)$$

$$= 10m(54n-11).$$

**Theorem 4** The augmented Zagreb index for $G = TNT_3[m,n]$ is given by

$$AZI(G) = \frac{16m}{7^3}(4374n - \frac{135949}{5^3}).$$

Proof. Using equation (5), Table 1 and simplifing, we have

$$AZI(G) = \sum_{uv\in E(G)} [\frac{d_u d_v}{d_u + d_v - 2}]^3$$

$$= 4m(2)^3 + 4m(\frac{12}{5})^3 + 4m(2)^3 - 10m(\frac{18}{7})^3 + 12mn(\frac{18}{7})^3$$

$$= \frac{16m}{7^3}(4374n - \frac{135949}{5^3}).$$

**Theorem 5** The first and second multiple Zagreb indices for $G = TNT_3[m,n]$ are given by

$$PM_1(G) = 2^{2m(2n+7)} \times 3^{6m(2n-1)}$$

and

$$PM_2(G) = 2^{6m(2n+3)} \times 3^{12m(2n-1)}.$$

Proof. Using equation (9) and Table 2, we get

$$PM_1(G) = \prod_{v\in V(G)} (d_v)^2$$

$$= (4)^{4m} \times (9)^{4mn-2n} \times (16)^{2m} \times (36)^{2mn-m}.$$

Which after simplification gives

$$PM_1(G) = 2^{2m(2n+7)} \times 3^{6m(2n-1)}.$$

Similarly, using equation (10) and Table 1 and after simplification, we have

$$PM_2(G) = \prod_{uv\in E(G)} d_u d_v$$

$$= (8)^{4m} \times (12)^{4m} \times (12)^{4m} \times (18)^{12mn-10m}$$

$$= 2^{6m(2n+3)} \times 3^{12m(2n-1).}$$

**Lemma 2** The Narumi-Katayama index for $G = TNT_3[m,n]$ is given by

$$NK(G) = 2^{m(2n+7)} \times 3^{3m(2n-1)}.$$

Proof. Using relation, $NK(G) = \sqrt{PM_1(G)}$ and Theorem 5, we get

$$NK(G) = \sqrt{2^{2m(2n+7)} \times 3^{6m(2n-1)}}$$

$$= 2^{m(2n+7)} \times 3^{3m(2n-1).}$$

**Theorem 6** The first Zagreb polynomial for $G = TNT_3[m,n]$ is given by

$$ZG_1(G,x) = 2mx^6[2+2x+2x^2+(6n-5)x^3].$$

Proof. Using equation (11) and Table 1, we have

$$ZG_1(G,x) = \sum_{uv\in E(G)} x^{d_u+d_v}$$

$$= 4mx^6 + 4mx^7 + 4mx^8 + (12mn-10m)x^9$$

$$= 2mx^6[2+2x+2x^2+(6n-5)x^3].$$

**Theorem 7** The second Zagreb polynomial for $G = TNT_3[m,n]$ is given by

$$ZG_2(G,x) = 2mx^8[2+4x^4+(6n-5)x^{10}].$$

Proof. Using equation (12) and Table 1, we get

$$ZG_2(G,x) = \sum_{uv\in E(G)} x^{d_u d_v}$$

$$= 4mx^8 + 4mx^{12} + 4mx^{12} + (12mn-10m)x^{18}$$

$$= 2mx^8[2+4x^4+(6n-5)x^{10}].$$

## ZAGREB INDICES AND ZAGREB POLYNOMIALS FOR SIX-LAYERED SINGLE-WALLED TITANIA NANOTUBE

The graph of six-layered single-walled titania nanotube can be viewed as in Figure 2. We denote the 2-parametric chemical graph of six-layered single-walled titania nanotube as $TNT_6[m,n]$. It is defined periodically as shown in Figure 2, where $m$ and $n$ are number of titanium atoms in each column and each row respectively.

The size of $TNT_6[m,n]$ is $20mn+2m$. There are six kinds of edges corresponding to their degrees of end vertices. Table 3 shows such an edge partition of edge set of $TNT_6[m,n]$.

The order of $TNT_6[m,n]$ is $12mn+4m$. There are four kinds of edges in the set $V(G)$ corresponding to their degrees.

Table 4 shows such a partition of the set $V(G)$ of $TNT_6[m,n]$.

The following theorems exhibit the Zagreb indices and Zagreb polynomials for this nanotube.

**Theorem 8** The reduced second Zagreb index for $G = TNT_6[m,n]$ is given by

$$RM_2(G) = 4m(32n-11).$$

Proof. Using equation (4) and Table 3, we get

$$RM_2(G) = \sum_{uv\in E(G)} (d_u - 1)\times(d_v - 1)$$

$$= 2m(1)(1) + 2m(1)(2) + 6m(1)(3) + 2m(2)(3) + 8mn(1)(4) + 2m(6n-5)(2)(4).$$

After simplification, we get the required result, $RM_2(G) = 4m(32n-11)$.

**Theorem 9** The third Zagreb index $G = TNT_6[m,n]$ is given by

$$M_3(G) = 4m(290n-61).$$

Proof. Using equation (5) and Table 3, we get

$$M_3(G) = \sum_{uv\in E(G)} (d_u + d_v)^2$$

$$= 2m(2+2)^2 + 2m(2+3)^2 + 6m(2+4)^2 + 2m(3+4)^2 + 8mn(2+5)^2 + 2m(6n-5)\times(3+5)^2.$$

Which after simplification gives us, $M_3(G) = 4m(290n-61)$.

**Theorem 10** The F-index for $G = TNT_6[m,n]$ is given by

$$F(G) = 128m(5n-1).$$

Proof. Using entries from Table 3, in equation (3), we have

$$F(G) = \sum_{uv\in E(G)} [(d_u)^2 + (d_v)^2]$$

$$= 2m(4+4) + 2m(4+9) + 6m(4+16) + 2m(9+16) + 8mn(4+25) + 2m(6n-5)(9+25).$$

Which after simplification gives us, $F(G) = 128m(5n-1)$.

**Theorem 11** The augmented Zagreb index $G = TNT_6[m,n]$ is given by

$$AZI(G) = \frac{m}{4}\left(1006n - \frac{29101}{5^3}\right).$$

Proof. Using entries from Table 3, in equation (5), we have

$$AZI(G) = \sum_{uv\in E(G)} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3$$

$$= 2m\left[\frac{(2)(2)}{2+2-2}\right]^3 + 2m\left[\frac{(2)(3)}{2+3-2}\right]^3 + 6m\left[\frac{(2)(4)}{2+4-2}\right]^3 + 8mn\left[\frac{(2)(5)}{2+5-2}\right]^3 + 2m\left[\frac{(3)(4)}{3+4-2}\right]^3 + 2m(6n-5)\left[\frac{(3)(5)}{3+5-2}\right]^3.$$

Which after simplification gives us, $AZI(G) = \frac{m}{4}\left(1006n - \frac{29101}{5^3}\right)$.

**Theorem 12** The Narumi-Katayama index for $G = TNT_6[m,n]$ is given by

$$NK(G) = 2^{2m(2n+5)} \times (15)^{2m(2n-1)}.$$

Proof. Using entries from Table 4, in equation (8), we have

$$NK(G) = \prod_{v\in V(G)} d_v$$

$$= 2^{4mn+6m} \times 3^{4mn-2m} \times 4^{2m} \times 5^{4mn-2m}$$

$$= 2^{2m(2n+5)} \times (15)^{2m(2n-1)}.$$

**Theorem 13** The first Zagreb polynomial for $G = TNT_6[m,n]$ is given by

$$ZG_1(G,x) = 2mx^4[1 + x + 3x^2 + (4n+1)x^3 + (6n-5)x^4].$$

Proof. Using entries from Table 3, in equation (11), we have

$$ZG_1(G,x) = \sum_{uv\in E(G)} x^{d_u + d_v}$$

$$= 2mx^4 + 2mx^5 + 6mx^6 + 2mx^7 + 8mnx^7 + (12mn - 10m)x^8$$

$$= 2mx^4[1 + x + 3x^2 + (4n+1)x^3 + (6n-5)x^4].$$

**Theorem 14** The second Zagreb polynomial for $G = TNT_6[m,n]$ is given by

$$ZG_2(G,x) = 2mx^4[1 + x^2 + 3x^4 + 4nx^6 + x^8 + (6n-5)x^{11}].$$

Proof. Using entries from Table 4, in equation (12), we have

$$ZG_2(G,x) = \sum_{uv\in E(G)} x^{d_u d_v}$$

$$= 2mx^4 + 2mx^6 + 6mx^8 + 2mx^{12} + 8mnx^{10} + (12mn - 10m)x^{15}$$

$$= 2mx^4[1 + x^2 + 3x^4 + 4nx^6 + x^8 + (6n-5)x^{11}].$$

## CONCLUSION AND GENERAL REMARKS

In this paper, we have conducted the study of Zagreb indices and Zagreb polynomials for the single-walled titania nanotubes. We have computed the exact formulae of Zagreb indices and Zagreb polynomials for the single-walled titania nanotubes. Various graph-theoretic parameters and certain distance based and counting related topological descriptors for these nanotubes an be considered for future study.

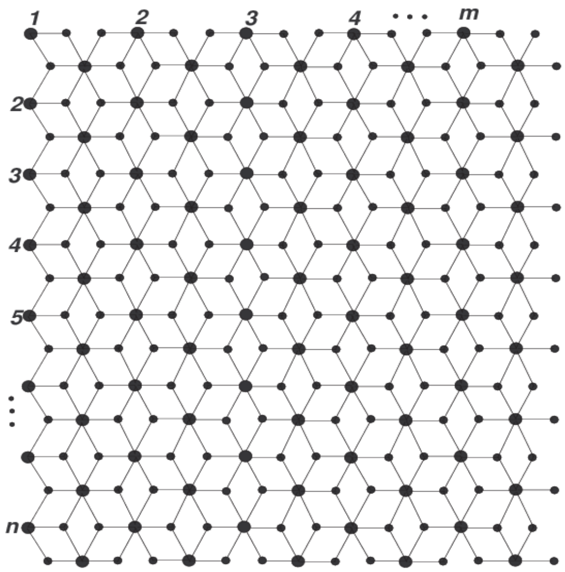


**Figure 1: The graph of three-layered single-walled titania nanotue**

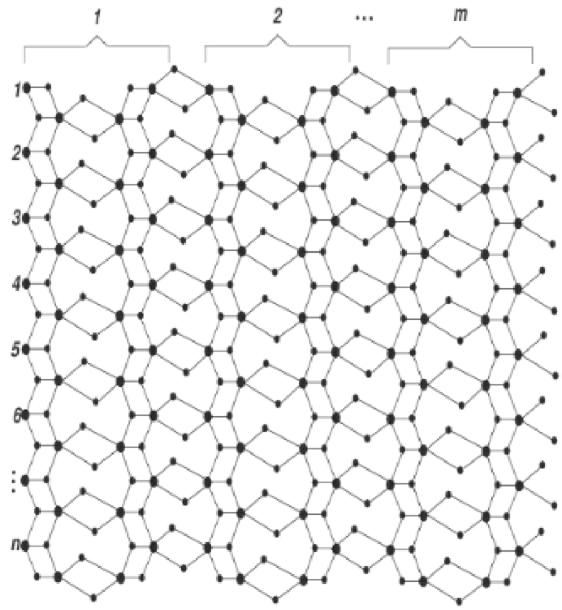


**Figure 2: The graph of six-layered single-walled titania nanotube**

**Table 1: Edge partition of edge set of $TNT_3[m,n]$**

| $(d_u,d_v)$ | (2,4) | (3,4) | (2,6) | (3,6) |
|---|---|---|---|---|
| Number of Edges | $4m$ | $4m$ | $4m$ | $2m(6n-5)$ |

**Table 2: The partition of $V(G)$ of $TNT_3[m,n]$**

| $d_v$ | 2 | 3 | 4 | 6 |
|---|---|---|---|---|
| Number of Vertices | $4m$ | $4mn-2m$ | $2m$ | $2mn-m$ |

**Table 3: Edge partition of edge set of $TNT_6[m,n]$**

| $(d_u,d_v)$ | (2,2) | (2,3) | (2,4) | (2,5) |
|---|---|---|---|---|
| Number of Edges | $2m$ | $2m$ | $6m$ | $8mn$ |
| $(d_u,d_v)$ | (3,4) | (3,5) | | |
| Number of Edges | $2m$ | $2m(6n-5)$ | | |

**Table 4: The partition of V(G) of $TNT_6[m,n]$**

| $d_v$ | 2 | 3 | 4 | 5 |
|---|---|---|---|---|
| Number of Vertices | $4mn+6m$ | $4mn-2m$ | $2m$ | $4mn-2m$ |

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