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3层和6层单壁二氧化钛纳米管的乘法萨格勒布指数

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摘要：由于二氧化钛在催化、气体传感和耐腐蚀材料生产中的广泛应用，使其成为目前研究最为广泛的纳米结构之一，而萨格勒布指数又是该研究中最为重要的拓扑指数. 因此，计算了3层和6层单壁二氧化钛纳米管的第1和第2广义乘法Zagreb指数，同时还从广义的第1和第2乘法Zagreb指数中恢复了第1和第2乘法Zagreb指数.

关键词：二氧化钛；纳米管；拓扑指数；乘法萨格勒布指数
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Multiplicative Zagreb Indices for the Three Layered and Six Layered Single-Walled Titania Nanotubes

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Abstract: Titania is one of the most comprehensively studied nanostructures due to the widespread applications in the production of catalytic, gas sensing, and corrosion-resistant materials. Zagreb indices are the most important topological indices, so we computed first and second generalized multiplicative Zagreb indices for the three and six layered single-walled Titania nanotubes. We also recovered first and second multiplicative Zagreb indices from the generalized first and second multiplicative Zagreb indices.

Key words: TiO_2; Nanotube; topological index; multiplicative Zagreb index

Titania, TiO_2, attracts considerable technological interest due to its unique properties in biology, optics, electronics, and photo-chemistry[1]. Recent experimental studies show that titania nanotubes (NTs) improve TiO_2 bulk properties for photocatalysis, hydrogen-sensing, and photo-voltaic applications[2]. Titanium nanotubes have been observed in two types of morphologies: single-walled titanium (SW TiO_2) nanotubes and multi-walled (MW TiO_2) nanotubes[3]. Here, we are interested only in single-walled TiO_2 nanotubes because we consider their chemical graphs to work on molecular descriptors. Titania nanotubes are formed by rolling up the stoichiometric two-periodic (2D) sheets cut from the energetically stable anatase surface.

In applied mathematics, chemical reaction network theory was initiated in 1960s and got huge attraction of researcher because this theory is used to model the chemical system phenomena's. This theory is applicable in theoretical and bio-chemistry.

Another interesting field of research is cheminformatics. In this study, topological indices together with quantitative structure-activity (QSAR) and Structure-property (QSPR) relationships guess different properties of chemical structures.

The area of research in chemistry in which mathematics is used to deal with the problems of chemistry is named as Mathematical Chemistry. For example, graph theory is a mathematical tool which is used to model the chemical structure and with the help of graph theoretical technics, one can obtain information about different chemical structures by using symmetry present in that structure. This particular branch of Mathematical Chemistry is known as

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Chemical Graph Theory[4].

The union of dots (vertices) and lines (edges) is called a graph and is denoted by G. The graph G is said to be connected if all of its vertices have connection between them. By degree of a vertex v, we mean the number of vertices at distance one from v and is represented by d_v.

Now, we give definitions of multiplicative Zagreb indices. Throughout this paper G denotes the connected graph without loops and multiple edges.

The first and second generalized multiplication Zagreb indices are defined as:

$$GMZ_1^{\alpha}(G) = \prod_{ij \in E(G)} (d_i + d_j)^{\alpha}$$

and

$$GMZ_2^{\alpha}(G) = \prod_{ij \in E(G)} (d_i \times d_j)^{\alpha}$$

respectively.

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respectively.

In this paper, we computed multiplicative three and six layered single-walled Titania Nanotubes.

1 Multiplicative Zagreb Indices of Three Layered Single-Walled Titania Nanotubes

Three layered single-walled Titania Nanotube is denoted by $TNT_3[m,n]$ and the molecular graph is given in Figure 1.

The Table 1 contains the edge partition of $TNT_3[m,n]$ based on the degree of end vertices.

Table 1 Edge Partition of $TNT_3[m, n]$

(d_i, d_j) Where $ij \in E(G)$	Number of Edges
(2,4)	$4m$
(3,4)	$4m$
(2,6)	$4m$
(3,6)	$2m(6n-5)$

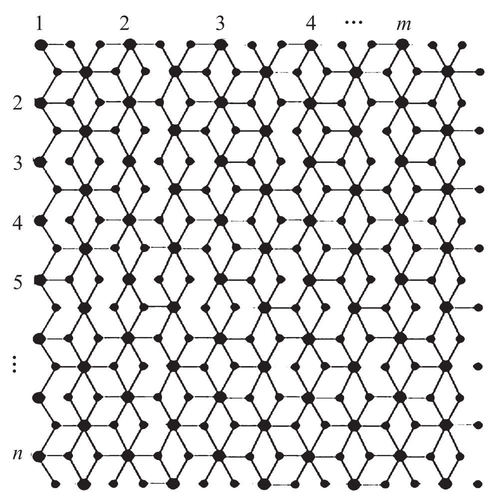

Figure 1 Graph of $TNT_3[m, n]$

Theorem 1 Let G be the graph of three layered single-walled Titania Nanotube, then we have:

$$GMZ_1^{\alpha}(G) = 2^{16\alpha m} \times 3^{8\alpha m(3n-2)} \times 7^{4\alpha m}.$$

Proof Using edge partition from Table 1, we have following computations for the first generalized multiplication Zagreb index:

$$\begin{aligned}
GMZ_1^{\alpha}(G) &= \prod_{ij \in E(G)} (d_i + d_j)^{\alpha} \\
&= \prod_{ij \in E_1(G)} (d_i + d_j)^{\alpha} \times \prod_{ij \in E_2(G)} (d_i + d_j)^{\alpha} \times \prod_{ij \in E_3(G)} (d_i + d_j)^{\alpha} \times \prod_{ij \in E_4(G)} (d_i + d_j)^{\alpha} \\
&= \prod_{ij \in E_1(G)} (2+4)^{\alpha} \times \prod_{ij \in E_2(G)} (3+4)^{\alpha} \times \prod_{ij \in E_3(G)} (2+6)^{\alpha} \times \prod_{ij \in E_4(G)} (3+6)^{\alpha} \\
&= (6^{\alpha})^{|ij \in E_1(G)|} \times (7^{\alpha})^{|ij \in E_2(G)|} \times (8^{\alpha})^{|ij \in E_3(G)|} \times (9^{\alpha})^{|ij \in E_4(G)|} \\
&= (6^{\alpha})^{4m} \times (7^{\alpha})^{4m} \times (8^{\alpha})^{4m} \times (9^{\alpha})^{2m(6n-5)}
\end{aligned}$$

$$= 2^{16\alpha m} \times 3^{8\alpha m(3n-2)} \times 7^{4\alpha m}.$$

Theorem 2 Let G be the graph of three layered single-walled Titania Nanotube, then we have:

$$GMZ_2^\alpha(G) = 2^{6\alpha m(2n-3)} \times 3^{12\alpha m(2n-1)}.$$

Proof Using edge partition from Table 1, we have following computations for the second generalized multiplication Zagreb index:

$$\begin{aligned} GMZ_2^\alpha(G) &= \prod_{ij\in E(G)} (d_i \times d_j)^\alpha \\ &= \prod_{ij\in E_1(G)} (d_i \times d_j)^\alpha \times \prod_{ij\in E_2(G)} (d_i \times d_j)^\alpha \times \prod_{ij\in E_3(G)} (d_i \times d_j)^\alpha \times \prod_{ij\in E_4(G)} (d_i \times d_j)^\alpha \\ &= \prod_{ij\in E_1(G)} (2\times 4)^\alpha \times \prod_{ij\in E_2(G)} (3\times 4)^\alpha \times \prod_{ij\in E_3(G)} (2\times 6)^\alpha \times \prod_{ij\in E_4(G)} (3\times 6)^\alpha \\ &= (8^\alpha)^{|ij\in E_1(G)|} \times (12^\alpha)^{|ij\in E_2(G)|} \times (12^\alpha)^{|ij\in E_3(G)|} \times (18^\alpha)^{|ij\in E_4(G)|} \\ &= (8^\alpha)^{4m} \times (12^\alpha)^{4m} \times (12^\alpha)^{4m} \times (18^\alpha)^{2m(6n-5)} \\ &= 2^{6\alpha m(2n-3)} \times 3^{12\alpha m(2n-1)}. \end{aligned}$$

Theorem 3 Let G be the graph of three layered single-walled Titania Nanotube, then we have:

$$MZ_1(G) = 2^{16m} \times 3^{8m(3n-2)} \times 7^{4m}.$$

Proof The result can be obtained immediately from Theorem 1.

Theorem 4 Let G be the graph of three layered single-walled Titania Nanotube, then we have:

$$MZ_2(G) = 2^{6m(2n-3)} \times 3^{12m(2n-1)}.$$

Proof The result can be obtained immediately from Theorem 2.

2 Multiplicative Zagreb Indices of Six Layered Single-Walled Titania Nanotubes

Let $TNT_6[m,n]$ be the six layered single-walled Titania Nanotube as shown in Figure 2.

The edge partition of $TNT_6[m,n]$ based on the degree of end vertices is given in Table 2.

Table 2 Edge Partition of $TNT_6[m, n]$

(d_i, d_j) Where $ij \in E(G)$	Number of Edges
(2,2)	$2m$
(2,3)	$2m$
(2,4)	$6m$
(2,5)	$8mn$
(3,4)	$2m$
(3,5)	$2m(6n-5)$

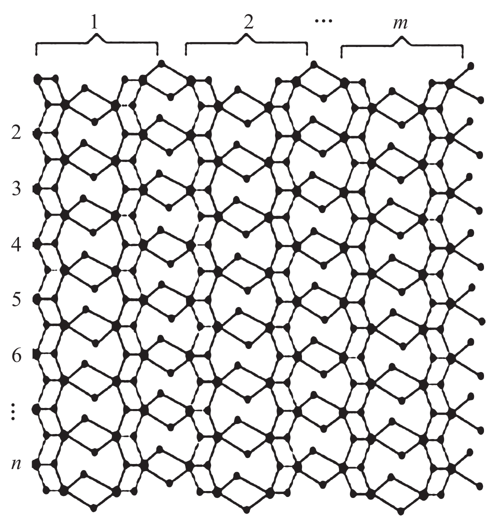

Figure 2 Graph of Six-Layered Single-Walled Titania Nanotube

Theorem 5 Let G be the graph of six layered single-walled Titania Nanotube, then we have:

$$GMZ_1^\alpha(G) = 2^{4\alpha m(9n-5)} \times 3^{6\alpha m} \times 5^{2\alpha m} \times 7^{2\alpha m(4n+1)}.$$

Proof Using edge partition from Table 2, we have following computations for the first generalized multiplication Zagreb index:

$$\begin{aligned} GMZ_1^\alpha(G) &= \prod_{ij\in E(G)} (d_i + d_j)^\alpha \\ &= \prod_{ij\in E_1(G)} (d_i + d_j)^\alpha \times \prod_{ij\in E_2(G)} (d_i + d_j)^\alpha \times \prod_{ij\in E_3(G)} (d_i + d_j)^\alpha \times \prod_{ij\in E_4(G)} (d_i + d_j)^\alpha \times \prod_{ij\in E_5(G)} (d_i + d_j)^\alpha \\ &\quad \times \prod_{ij\in E_6(G)} (d_i + d_j)^\alpha \\ &= \prod_{ij\in E_1(G)} (2+2)^\alpha \times \prod_{ij\in E_2(G)} (2+3)^\alpha \times \prod_{ij\in E_3(G)} (2+4)^\alpha \times \prod_{ij\in E_4(G)} (2+5)^\alpha \times \prod_{ij\in E_5(G)} (3+4)^\alpha \times \end{aligned}$$

$$\prod_{ij\in E_6(G)}(3+5)^{\alpha}$$
$$=(4^{\alpha})^{|ij\in E_1(G)|}\times(5^{\alpha})^{|ij\in E_2(G)|}\times(6^{\alpha})^{|ij\in E_3(G)|}\times(7^{\alpha})^{|ij\in E_4(G)|}\times(7^{\alpha})^{|ij\in E_5(G)|}\times(8^{\alpha})^{|ij\in E_6(G)|}$$
$$=(4^{\alpha})^{2m}\times(5^{\alpha})^{2m}\times(6^{\alpha})^{6m}\times(7^{\alpha})^{8mn}\times(7^{\alpha})^{2m}\times(8^{\alpha})^{2m(6n-5)}$$
$$=2^{4\alpha m(9n-5)}\times 3^{6\alpha m}\times 5^{2\alpha m}\times 7^{2\alpha m(4n+1)}.$$

Theorem 6 Let G be the graph of six layered single-walled Titania Nanotube, then we have:

$$GMZ_2^{\alpha}(G)=2^{2\alpha m(4n+13)}\times 3^{2\alpha m(6n-3)}\times 5^{10\alpha m(2n-1)}.$$

Proof Using edge partition from Table 2, we have following computations for the second generalized multiplication Zagreb index:

$$GMZ_2^{\alpha}(G)=\prod_{ij\in E(G)}(d_i\times d_j)^{\alpha}$$
$$=\prod_{ij\in E_1(G)}(d_i\times d_j)^{\alpha}\times\prod_{ij\in E_2(G)}(d_i\times d_j)^{\alpha}\times\prod_{ij\in E_3(G)}(d_i\times d_j)^{\alpha}\times\prod_{ij\in E_4(G)}(d_i\times d_j)^{\alpha}\times\prod_{ij\in E_5(G)}(d_i\times d_j)^{\alpha}\times\prod_{ij\in E_6(G)}(d_i\times d_j)^{\alpha}$$
$$=\prod_{ij\in E_1(G)}(2\times 2)^{\alpha}\times\prod_{ij\in E_2(G)}(2\times 3)^{\alpha}\times\prod_{ij\in E_3(G)}(2\times 4)^{\alpha}\times\prod_{ij\in E_4(G)}(2\times 5)^{\alpha}\times\prod_{ij\in E_5(G)}(3\times 4)^{\alpha}\times\prod_{ij\in E_6(G)}(3\times 5)^{\alpha}$$
$$=(4^{\alpha})^{|ij\in E_1(G)|}\times(6^{\alpha})^{|ij\in E_2(G)|}\times(8^{\alpha})^{|ij\in E_3(G)|}\times(10^{\alpha})^{|ij\in E_4(G)|}\times(12^{\alpha})^{|ij\in E_5(G)|}\times(15^{\alpha})^{|ij\in E_6(G)|}$$
$$=(4^{\alpha})^{2m}\times(6^{\alpha})^{2m}\times(8^{\alpha})^{6m}\times(10^{\alpha})^{8mn}\times(12^{\alpha})^{2m}\times(15^{\alpha})^{2m(6n-5)}$$
$$=2^{2\alpha m(4n+13)}\times 3^{2\alpha m(6n-3)}\times 5^{10\alpha m(2n-1)}.$$

Theorem 7 Let G be the graph of six layered single-walled Titania Nanotube, then we have:

$$MZ_1(G)=2^{4m(9n-5)}\times 3^{6m}\times 5^{2m}\times 7^{2m(4n+1)}.$$

Proof This result can be obtained immediately from Theorem 5.

Theorem 8 Let G be the graph of six layered single-walled Titania Nanotube, then we have:

$$MZ_2(G)=2^{2m(4n+13)}\times 3^{2m(6n-3)}\times 5^{10m(2n-1)}.$$

Proof This result can be obtained immediately form Theorem 6.

3 Conclusions

In this paper, we computed generalized version of first and second multiplicative Zagreb indices for two important classes of Nanotubes. From the computed results, we recover first and second multiplicative Zagreb indices. One can also recover some other versions of multiplicative indices from our results, for example, multiplicative first and second Harmonic indices and multiplicative sum and product connectivity indices can also be obtained from our results.

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