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M-Polynomials and Topological Indices of Titania Nanotubes

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Abstract: Titania is one of the most comprehensively studied nanostructures due to their widespread applications in the production of catalytic, gas sensing, and corrosion-resistant materials. M-polynomial of nanotubes has been vastly investigated, as it produces many degree-based topological indices, which are numerical parameters capturing structural and chemical properties. These indices are used in the development of quantitative structure-activity relationships (QSARs) in which the biological activity and other properties of molecules, such as boiling point, stability, strain energy, etc., are correlated with their structure.

In this report, we provide M-polynomials of single-walled titania (SW TiO_2) nanotubes and recover important topological degree-based indices to theoretically judge these nanotubes. We also plot surfaces associated to single-walled titania (SW TiO_2) nanotubes.

Keywords: degree-based topological index; Zagreb index; general randic index; symmetric division index; M-polynomial; titania nanotubes

1. Introduction

In chemical graph theory, molecular topology, and mathematical chemistry, a topological index, sometimes known as a connectivity index, is a type of a molecular descriptor which is calculated based on the molecular graph of a chemical compound. A large amount of chemical experiments require a determination of the chemical properties of new compounds and new drugs. Fortunately, the chemical-based experiments indicate that there is strong inherent relationship between the chemical characteristics of chemical compounds and drugs and their molecular structures. Topological indices calculated for these chemical molecular structures can help us to understand the physical features, chemical reactivity, and biological activity.

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, which contains either six $(O - Ti - O - O - Ti - O)$ or three $(O - Ti - O)$ layers [4].

The $TNT_3\,[m, n]$ is the two-parametric chemical graph of three-layered titania nanotubes, where m and n represent the number of titanium atoms in each row and column, respectively (Figure 1). Big dots correspond to titanium atoms, whereas small dots correspond to oxygen atoms, and edges represent bonds.

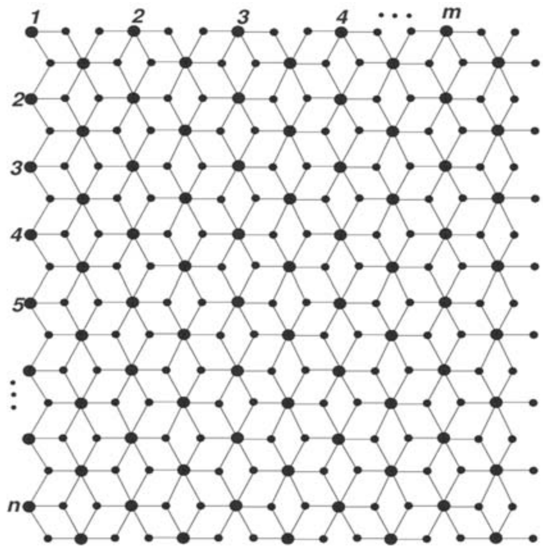

Figure 1. The graph of three-layered single-walled titania nanotubes.

$TNT_6\,[m, n]$ is the two-parametric chemical graph of a six-layered single-walled titania nanotube, where m and n represent the number of titanium atoms in each column and row, respectively (Figure 2). Here again, big dots correspond to titania atoms, small dots to oxygen, and edges to atomic bonds.

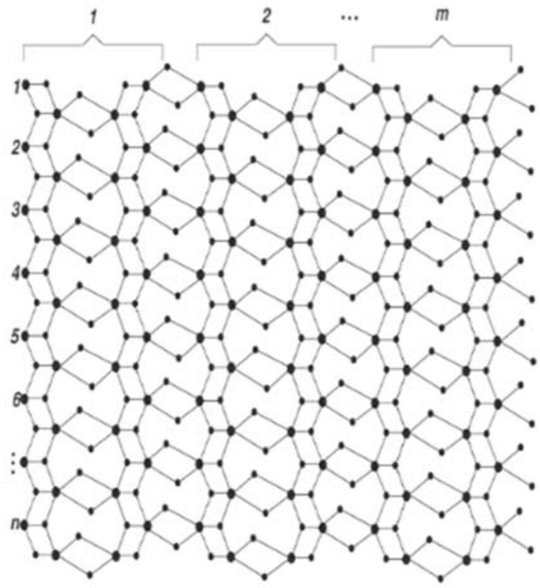

Figure 2. The graph of six-layered single walled titania nanotubes.

In order to engineer a nanotube endowed with a proposed property, one can have control over structural sensitive properties such as fracture toughness and yield stress. The topological index of a molecule structure can be considered as a non-empirical numerical quantity that quantifies the molecular structure and its branching pattern in many ways. In this point of view, the topological index can be regarded as a score function that maps each molecular structure to a real number and is used as a descriptor of the molecule under testing.

The Wiener index is the first and most studied topological index and is defined as the sum of the distances between all pairs of vertices in G. For more details, see [5,6]. Zagreb indices were introduced by Gutman and Trinajstic [7]. The first Zagreb index $M_1(G)$ is defined as the sum of the squares of degrees of a graph G, and the second Zagreb index $M_2(G)$ is the sum of the product of all degrees corresponding to each edge in G [7]. The second modified Zagreb index is defined by ${}^{m}M_2(G) = \sum_{uv \in E(G)} d_u d_v$, where d_u and d_v are the degrees of vertices u and v, respectively [8]. General Randic index of G is defined as the sum of $(d_u d_v)^{\alpha}$ over all edges uv of G, where d_u denotes the degree of vertex u of G, and $R_{\alpha}(G) = \sum_{uv \in E(G)} (d_u d_v)^{\alpha}$, where α is an arbitrary real number [9]. Symmetric division index is defined as $\sum_{uv \in E(G)} \left\{ \frac{\min(d_u,d_v)}{\max(d_u,d_v)} + \frac{\max(d_u,d_v)}{\min(d_u,d_v)} \right\}$. These indices can help to characterize the chemical and physical properties of molecules [7,9–20]. Most recently, Munir et al. computed M-polynomials and related topological indices for Bucktubes [11] and Nanostar dendrimers [19].

In the present article, we compute the closed forms of M-polynomials of single-walled titania nanotubes and represent them graphically using Mapple. As a consequence, we derived some topological degree-based indices. We start by defining the M-polynomial of a general graph [7]. It is important to mention that black titania nanotubes are used to control photo-catalysis and crystalline structures. These tubes have applications in nanotechnology, optics, and electronics. In these areas, computations of topological indices can predict properties of these tubes and avoid a large amount of chemical experiments.

Definition 1. *If $G = (V, E)$ is a graph where V denotes vertices and E represents edges of G. Let $d_v(G)$ represent the degree of v in graph G. Let $m_{ij}(G); i, j \geq 1$ be the number of edges $e = uv$ of G such that $\{d_u(G), d_v(G)\} = \{i, j\}$, which means the M-Polynomial of graph G is defined as*

$$M(G, x, y) = \sum_{i \leq j} m_{ij}(G) x^i y^j. \tag{1}$$

Topological indices are numerical parameters of a graph that characterize its topology and are usually graph-invariant. It describes the structure of molecules numerically. Topological indices are used in the development of qualitative structure activity relationships (QSARs). Some degree-based topological indices are derived from M-polynomials [21]. The following Table 1 relates these derivations.

Table 1. Derivations of degree-based indices

Topological Index	$f(x,y)$	Derivation from $M(G;x,y)$
First Zagreb	$x+y$	$(D_x + D_y)(M(G;x,y))\big\vert_{x=y=1}$
Second Zagreb	xy	$(D_x D_y)(M(G;x,y))\big\vert_{x=y=1}$
Second Modified Zagreb	$\frac{1}{xy}$	$(S_x S_y)(M(G;x,y))\big\vert_{x=y=1}$
General Randić $\alpha \in \mathbb{N}$	$(xy)^{\alpha}$	$(D_x^{\alpha} D_y^{\alpha})(M(G;x,y))\big\vert_{x=y=1}$
General Randić $\alpha \in \mathbb{N}$	$\frac{1}{(xy)^{\alpha}}$	$(S_x^{\alpha} S_y^{\alpha})(M(G;x,y))\big\vert_{x=y=1}$
Symmetric Division Index	$\frac{x^2+y^2}{xy}$	$(D_x S_y + S_x D_y)(M(G;x,y))\big\vert_{x=y=1}$

$D_x = \frac{\partial(f(x,y))}{\partial x}$; $D_y = \frac{\partial(f(x,y))}{\partial y}$; $S_x = \int_0^x \frac{f(t,y)}{t} dt$; $S_y = \int_0^y \frac{f(x,t)}{t} dt$.

2. Results

In this section, we use the symmetric structures of single-walled titania nanotubes to determine the M-polynomials and then derive topological indices for these tubes.

Proposition 1. *Let $TNT_3[m,n]$ be the three-layered single-walled titania nanotube. Therefore,* $M(TNT_3[m,n],x,y) = 4mx^2y^4 + 4mx^3y^4 + 4mx^2y^6 + 2m(6n-5)x^3y^6$.

Proof. Let $TNT_3[m,n]$ be the three-layered single-walled titania nanotube, where m and n are the number of titanium atoms in each row and column, respectively. The graph has $6mn + 3m$ number of vertices and $12mn + 2m$ edges. The following are the tables for the vertex and edge partitions of $TNT_3[m,n]$ nanotubes.

From Table 2, we see that there are four partitions, $V_{\{2\}} = \{v\epsilon TNT_3[m,n] | d_v = 2\}$, $V_{\{3\}} = \{v\epsilon TNT_3[m,n] | d_v = 3\}$, $V_{\{4\}} = \{v \int TNT_3[m,n] | d_v = 4\}$, and $V_{\{6\}} = \{v\epsilon TNT_3[m,n] | d_v = 6\}$ for the vertex set $V(TNT_3[m,n])$ with size $4m, 4mn-2m, 2m$ and $2mn-m$, respectively.

As we can see in Table 3, the edge set of $TNT_3[m,n]$ can be written as

$$E_{\{2,4\}} = \{e = uv \in E(TNT_3[m,n]) | d_u = 2,\ d_v = 4\} \to \left|E_{\{2,4\}}\right| = 4m, \tag{2}$$

$$E_{\{2,6\}} = \{e = uv \in E(TNT_3[m,n]) | d_u = 2,\ d_v = 6\} \to \left|E_{\{2,6\}}\right| = 4m, \tag{3}$$

$$E_{\{3,4\}} = \{e = uv \in E(TNT_3[m,n]) | d_u = 3,\ d_v = 4\} \to \left|E_{\{3,4\}}\right| = 4m\ , \tag{4}$$

and

$$E_{\{3,6\}} = \{e = uv \in E(TNT_3[m,n]) | d_u = 3,\ d_v = 6\} \to \left|E_{\{3,6\}}\right| = 2m(6n-5)\,. \tag{5}$$

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 $TNT_3[m,n]$.

$(d_u,\ d_v)$	**(2 , 4)**	**(3 , 4)**	**(2 , 6)**	**(3 , 6)**
Number of edges	$4m$	$4m$	$4m$	$2m(6n-5)$

Thus, the M-polynomial of $TNT_3[m,n]$ is

$$\begin{aligned} M(TNT_3[m,n],x,y) &= \sum_{i\le j} m_{ij}(TNT_3[m,n])\,x^iy^j \\ &= \sum_{2\le 4} m_{24}(TNT_3[m,n])\,x^2y^4 + \sum_{3\le 4} m_{34}(TNT_3[m,n])\,x^3y^4 \\ &\quad + \sum_{2\le 6} m_{26}(TNT_3[m,n])\,x^2y^6 + \sum_{3\le 6} m_{36}(TNT_3[m,n])\,x^3y^6 \\ &= \sum_{uv\in E_{\{2,4\}}} m_{24}(TNT_3[m,n])\,x^2y^4 + \sum_{uv\in E_{\{3,4\}}} m_{34}(TNT_3[m,n])\,x^3y^4 \\ &\quad + \sum_{uv\in E_{\{2,6\}}} m_{26}(TNT_3[m,n])\,x^2y^6 + \sum_{uv\in E_{\{3,6\}}} m_{36}(TNT_3[m,n])\,x^3y^6 \\ &= \left|E_{\{2,4\}}\right| x^2y^4 + \left|E_{\{3,4\}}\right| x^3y^4 + \left|E_{\{2,6\}}\right| x^2y^6 + \left|E_{\{3,6\}}\right| x^3y^6 \\ &= 4mx^2y^4 + 4mx^3y^4 + 4mx^2y^6 + 2m(6n-5)\,x^3y^6 \end{aligned} \tag{6}$$

Proposition 2. *Let $TNT_6[m,n]$ be the six-layered single walled titania nanotube. Therefore,* $M(TNT_6[m,n],x,y) = 2mx^2y^2 + 2mx^2y^3 + 6mx^2y^4 + 8mnx^2y^5 + 2mx^3y^4 + 2m(6n-5)x^3y^5$.

Proof. Let $TNT_6[m,n]$ be the six-layered single walled titania nanotube, where m and n are the number of titanium atoms in each row and column, respectively. The graph has $12mn + 4m$ number of vertices and $20mn + 2m$ edges. Table 4 provides the edge partitions of $TNT_6[m,n]$, and Table 5 provides Vertex partitions.

Table 4. Edge partition of edge set of $TNT_6[m,n]$.

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

Table 5. The partition of $V(G)$ of $TNT_6[m,n]$.

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

From Table 4, we see that the partitions of $V(G)$ of $TNT_6[m,n]$ are $V_{\{2\}} = \{v\epsilon TNT_6[m,n] | d_v = 2\}$, $V_{\{3\}} = \{v\epsilon TNT_6[m,n] | d_v = 3\}$, $V_{\{4\}} = \{v\epsilon TNT_6[m,n] | d_v = 4\}$, and $V_{\{5\}} = \{v\epsilon TNT_6[m,n] | d_v = 5\}$ for the vertex set $V(TNT_6[m,n])$ with size $4mn + 6m$, $4mn - 2m$, $2m$ and $4mn - 2m$, respectively. From Table 5, the edge set of $TNT_6[m,n]$ can be written as

$$E_{\{2,2\}} = \{e = uv \in E(TNT_6[m,n]) | d_u = 2, d_v = 2\} \to \left|E_{\{2,2\}}\right| = 2m, \tag{7}$$

$$E_{\{2,3\}} = \{e = uv \in E(TNT_6[m,n]) | d_u = 2, d_v = 3\} \to \left|E_{\{2,3\}}\right| = 2m, \tag{8}$$

$$E_{\{2,4\}} = \{e = uv \in E(TNT_6[m,n]) | d_u = 2, d_v = 4\} \to \left|E_{\{2,4\}}\right| = 6m, \tag{9}$$

$$E_{\{2,5\}} = \{e = uv \in E(TNT_6[m,n]) | d_u = 2, d_v = 5\} \to \left|E_{\{2,5\}}\right| = 8mn, \tag{10}$$

$$E_{\{3,4\}} = \{e = uv \in E(TNT_6[m,n]) | d_u = 3,\ d_v = 4\} \to \left|E_{\{3,4\}}\right| = 2m\ , \tag{11}$$

and

$$E_{\{3,5\}} = \{e = uv \in E(TNT_6[m,n]) | d_u = 3,\ d_v = 5\} \to \left|E_{\{3,5\}}\right| = 2m(6n-5)\,. \tag{12}$$

$$\begin{aligned}
M(TNT_6[m,n],x,y) &= \sum_{i\le j} m_{ij}(TNT_3[m,n])\,x^iy^j \\
&= \sum_{2\le 2} m_{22}(TNT_6[m,n])\,x^2y^2 + \sum_{2\le 3} m_{23}(TNT_6[m,n])\,x^2y^3 \\
&+ \sum_{2\le 4} m_{24}(TNT_6[m,n])\,x^2y^4 + \sum_{2\le 5} m_{25}(TNT_6[m,n])\,x^2y^5 \\
&+ \sum_{3\le 4} m_{34}(TNT_6[m,n])\,x^3y^4 + \sum_{3\le 5} m_{35}(TNT_6[m,n])\,x^3y^5 \\
&= \sum_{uv\in E_{\{2,2\}}} m_{22}(TNT_6[m,n])\,x^2y^2 + \sum_{uv\in E_{\{2,3\}}} m_{23}(TNT_6[m,n])\,x^2y^3 \\
&+ \sum_{uv\in E_{\{2,4\}}} m_{24}(TNT_6[m,n])\,x^2y^4 + \sum_{uv\in E_{\{2,5\}}} m_{25}(TNT_6[m,n])\,x^2y^5. \\
&+ \sum_{uv\in E_{\{3,4\}}} m_{34}(TNT_6[m,n])\,x^3y^4 + \sum_{uv\in E_{\{3,5\}}} m_{35}(TNT_6[m,n])\,x^3y^5 \\
&= \left|E_{\{2,2\}}\right| x^2y^2 + \left|E_{\{2,3\}}\right| x^2y^3 + \left|E_{\{2,4\}}\right| x^2y^4 + \left|E_{\{2,5\}}\right| x^2y^5 \\
&+ \left|E_{\{3,4\}}\right| x^3y^4 + \left|E_{\{3,5\}}\right| x^{3646}y^5 \\
&= 2mx^2y^2 + 2mx^2y^3 + 6mx^2y^4 + 8mnx^2y^5 + 2mx^3y^4 + 2m(6n-5)\,x^3y^5
\end{aligned}\ . \tag{13}$$

The following results provide the computation of the topological indices of the three-layered and six-layered single-walled titania nanotubes.

Proposition 3. For the three-layered single-walled titania nanotube $TNT_3\,[m,n]$ we have

1 $M_1\,(TNT_3\,[m,n]) = 108mn - 6m$,
2 $M_2(TNT_3[m,n] = 2592m^2n^2 - 288m^2n + 8m^2$,
3 ${}^{m}M_2(TNT_3[m,n]) = 8m^2n^2 + 8m^2n + 2m^2$,
4 $R_a(G) = \left(2592m^2n^2 - 288m^2n + 8m^2\right)^{\alpha}$,
5 $R_a(G) = \left(8m^2n^2 + 8m^2n + 2m^2\right)^{\alpha}$,
6 $SDD(G) = 360m^2n^2 + 160m^2n - 10m^2$.

Proof. Let $f\,(x,y)$ be the M-polynomial of $TNT_3\,[m,n]$. Therefore,

$$f\,(TNT_3\,[m,n]\,;x,y) = 4mx^2y^4 + 4mx^3y^4 + 4mx^2y^6 + 2m\,(6n-5)\,x^3y^6, \tag{14}$$

$$D_x(f(x,y)) = 8mxy^4 + 12mx^2y^4 + 8mxy^6 + 6m(6n-5)x^2y^6, \tag{15}$$

$$D_y(f(x,y)) = 16mx^2y^3 + 16mx^3y^3 + 24mx^2y^5 + 12m(6n-5)x^3y^5, \tag{16}$$

$$S_x(f(x,y)) = 2mx^2y^4 + 4/3mx^3y^4 + 2mx^2y^6 + 2/3m(6n-5)x^3y^6, \tag{17}$$

$$S_y(f(x,y)) = mx^2y^4 + mx^3y^4 + 2/3mx^2y^6 + 1/3m(6n-5)x^3y^6, \tag{18}$$

$$D_y\,(f\,(TNT_3\,[m,n]\,;x,y))\big|_{x=y=1} = 72mn - 4m, \tag{19}$$

$$S_x\,(f\,(TNT_3\,[m,n]\,;x,y))\big|_{x=y=1} = 4mn + 2m, \tag{20}$$

$$S_y\,(f\,(TNT_3\,[m,n]\,;x,y))\big|_{x=y=1} = 2mn + m, \tag{21}$$

1 $M_1(TNT_3[m,n]) = (D_x + D_y)(M(G;x,y))\big|_{(x=y=1)} = 108mn - 6m$,
2 $M_2(TNT_3[m,n]) = (D_xD_y)(M(G;x,y))\big|_{(x=y=1)} = 2592m^2n^2 - 288m^2n + 8m^2$,
3 ${}^{m}M_2\,(TNT_3\,[m,n]) = (S_xS_y)\,(M\,(G;x,y))\big|_{x=y=1} = 8m^2n^2 + 8m^2n + 2m^2$,
4 $R_a(G) = (D_x^{\alpha}D_y^{\alpha})(M(G;x,y))\Big|_{x=y=1} = \left(2592m^2n^2 - 288m^2n + 8m^2\right)^{\alpha}$,
5 $R_a(G) = (S_x^{\alpha}S_y^{\alpha})(M(G;x,y))\Big|_{x=y=1} = \left(8m^2n^2 + 8m^2n + 2m^2\right)^{\alpha}$,
6 $SDD(G) = (D_xS_y + S_xD_y)(M(G;x,y))\big|_{x=y=1} = 360m^2n^2 + 160m^2n - 10m^2$.

Proposition 4. For the six-layered single-walled titania nanotube $TNT_6[m,n]$ we have

1 $M_1(TNT_6[m,n] = 152mn - 12m$,
2 $M_2(TNT_6[m,n] = 5200m^2n^2 - 816m^2n + 32m^2$,
3 ${}^{m}M_2\,(TNT_6\,[m,n]) = 32m^2n^2 + \frac{68}{3}m^2n + \frac{35}{9}m^2$,
4 $R_a(G) = \left(5200m^2n^2 - 816m^2n + 32m^2\right)^{\alpha}$,
5 $R_a(G) = \left(32m^2n^2 + 68/3m^2n + 35/9m^2\right)^{\alpha}$,
6 $SDD\,(G) = 1008m^2n^2 + 240m^2n - 12m^2$.

Proof. Let $f\,(x,y)$ be M-polynomial of $TNT_6\,[m,n]$. Therefore,

$$f\,(TNT_3\,[m,n]\,;x,y) = 2mx^2y^2 + 2mx^2y^3 + 6mx^2y^4 + 8mnx^2y^5 + 2mx^3y^4 + 2m\,(6n-5)\,x^3y^5, \tag{22}$$

$$D_x\,(f\,(x,y)) = 4mxy^2 + 4mxy^3 + 12mxy^4 + 16mnxy^5 + 6mx^2y^4 + 6m\,(6n-5)\,x^2y^5, \tag{23}$$

$$D_y\,(f\,(x,y)) = 4mx^2y + 6mx^2y^2 + 24mx^2y^3 + 40mnx^2y^4 + 8mx^3y^3 + 10m\,(6n-5)\,x^3y^4, \tag{24}$$

$$S_x\left(f\left(x,y\right)\right)=mx^2y^2+mx^2y^3+3mx^2y^4+4mnx^2y^5+\frac{2}{3}mx^3y^4+4mnx^3y^5-\frac{10}{3}mx^3y^5, \quad (25)$$

$$S_y\left(f\left(x,y\right)\right)=mx^2y^2+\frac{2}{3}mx^2y^3+\frac{3}{2}mx^2y^4+\frac{8}{5}mnx^2y^5+\frac{1}{2}mx^3y^4+\frac{12}{5}mnx^3y^5-2mx^3y^5, \quad (26)$$

$$D_x\left(f\left(TNT_3\left[m,n\right];x,y\right)\right)|_{x=y=1}=52mn-4m, \quad (27)$$

$$D_y\left(f\left(TNT_3\left[m,n\right];x,y\right)\right)|_{x=y=1}=100mn-8m, \quad (28)$$

$$S_x\left(f\left(TNT_3\left[m,n\right];x,y\right)\right)|_{x=y=1}=8mn+\frac{7}{3}m, \quad (29)$$

$$S_y\left(f\left(TNT_3\left[m,n\right];x,y\right)\right)|_{x=y=1}=4mn+\frac{5}{3}m, \quad (30)$$

1. $M_1\left(TNT_3\left[m,n\right]\right)=\left(D_x+D_y\right)\left(M\left(G;x,y\right)\right)\big|_{x=y=1}=152mn-12m,$
2. $M_2(TNT_3[m,n])=(D_xD_y)(M(G;x,y))\Big|_{(x=y=1)}=5200m^2n^2-816m^2n+32m^2,$
3. ${}^{m}M_2\left(TNT_3\left[m,n\right]\right)=\left(S_xS_y\right)\left(M\left(G;x,y\right)\right)\big|_{x=y=1}=32m^2n^2+\frac{68}{3}m^2n+\frac{35}{9}m^2,$
4. $R_a(G)=(D_x^{\alpha}D_y^{\alpha})(M(G;x,y))\Big|_{(x=y=1)}=(5200m^2n^2-816m^2n+32m^2)^{\alpha},$
5. $R_a(G)=(S_x^{\alpha}S_y^{\alpha})(M(G;x,y))\Big|_{(x=y=1)}=(32m^2n^2+68/3m^2n+35/9m^2)^{\alpha},$
6. $SDD(G)=(D_xS_y+S_xD_y)(M(G;x,y))\Big|_{(x=y=1)}=1008m^2n^2+240m^2n-12m^2.$

3. Conclusions

In this article, we computed the connectivity of titania nanotubes through degree-based topological indices. In Figures 3 and 4, we gave graphically representation of M-polynomial of 3-layered single walled titania nanotbes and 6-layered single walled titania nanotubes. The topological indices thus calculated for these titania nanotubes can help us to understand their physical features, chemical reactivity, and biological activities. From this point of view, topological indices can be regarded as a score function that maps each molecular structure to a real number and are used as descriptors of the molecule under testing. These results can also play a vital role in the determination of the significance of single-walled titania nanotubes in pharmaceutical industry [22,23]. In addition, a comparison between three- and six-layered titania nanotubes can be launched with the help of careful analysis of the above results. The methodology described above can be extended to emerging types of neontubes: aluminosilicate/aluminugerminate [20,24–26].

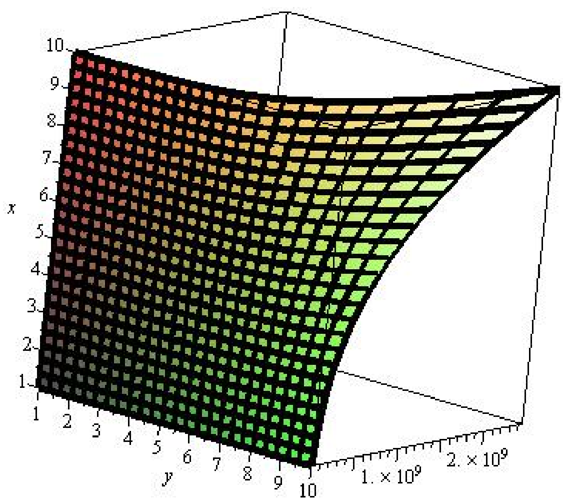

Figure 3. M-polynomial of 3-layered single walled titania nanotbes.

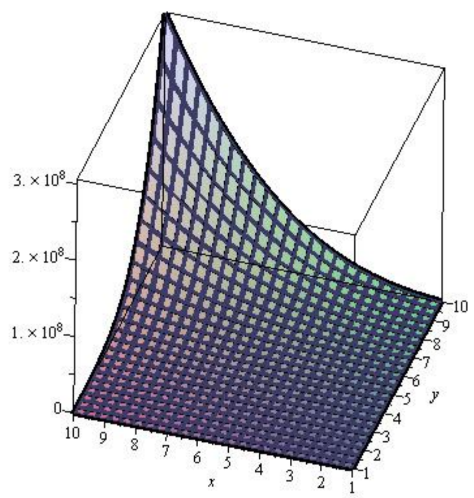

Figure 4. M-Polynomials of 6-layered single walled titania nanotubes.

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