M-Polynomials and Topological Indices of Titania Nanotubes

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Abstract: Titania are one of the most comprehensively studied nanostructures due to their widespread applications in production of catalytic, gas-sensing and corrosion-resistance materials [1]. 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 are correlated with their structure like boiling point, stability, strain energy etc of chemical compounds. In this report, we give M-polynomials of single-walled titania (SW TiO_2) nanotubes and recover important topological degree-based indices of them to judge theoretically these nanotubes. We also use Maple to plot surfaces associated to different types of single-walled titania (SW TiO_2) nanotubes.

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

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1. Introduction

In chemical graph theory, molecular topology, and mathematical chemistry, a topological index sometimes known as 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 determining 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, $Ti0_2$, attract considerable technological interests due to unique properties in biology, optics, electronics and photo-chemistry [2]. Recent experimental studies show that Titania nanotubes (NTs) improve $Ti0_2$ bulk properties for photocatalysis, hydrogen-sensing and photo-voltaic applications [3]. Various titanium nanotubes were observed in two types of morphologies:

multi- walled (MW) observed in two scroll like frequently containing various types of defects and impurities [4]. Titanium NTs have two forms, single-walled titanium (SW TiO_2) nanotubes and second is multi-walled (MW TiO_2) nanotubes. However 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 [5].

The $TNT_3[m,n]$ is the 2- parametric chemical graph of 3- layered Titania nanotubes, where m and n represent number of titanium atoms in each row and column respectively (fig. 1). Big dots correspond to Titanium atoms where as small dots are oxygen atoms and edges represent bonds.

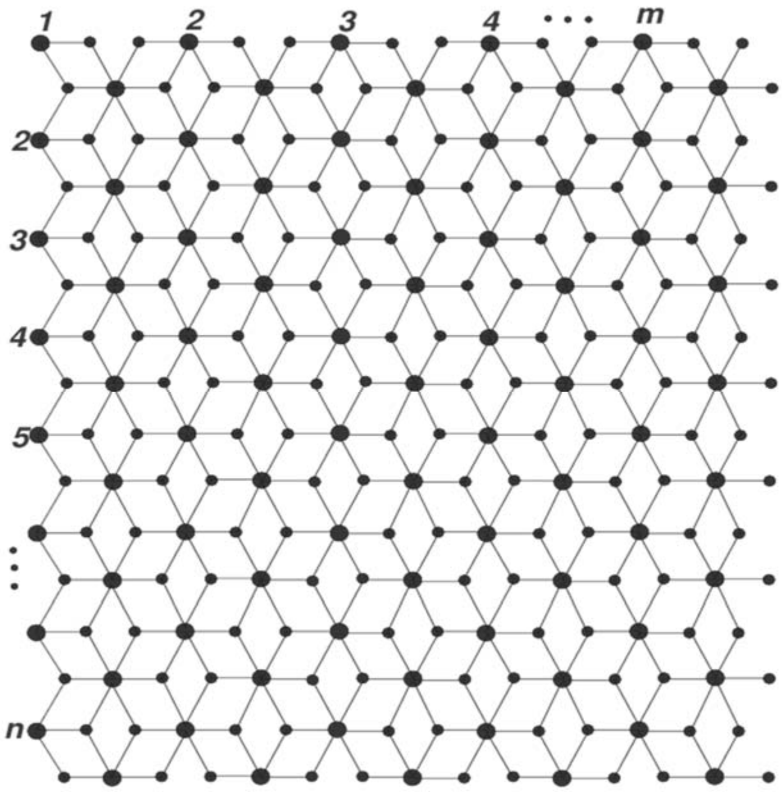

Fig 1: The graph of 3-layered single-walled Titania nanotubes

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

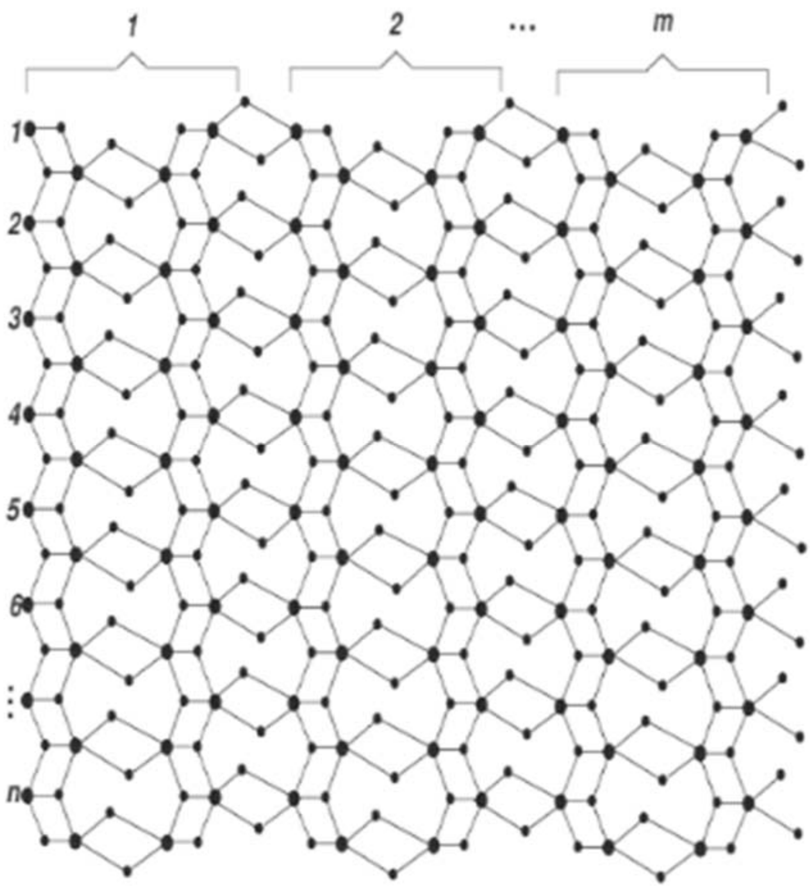

Fig 2: The graph of 6-layered single walled Titania nanotubes.

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

The Wiener index is originally the first and most studied topological index and is defined as the sum of distances between all pairs of vertices in G, for more details see [15,18]. Zagreb indices have been introduced by I. Gutman and N. Trinajstic [24]. First Zagreb index $M_1(G)$ is defined as sum of the squares of degrees of a graph G and second Zagreb $M_2(G)$ is sum of the product of all degrees corresponding to each edge in G see [24]. Second modified Zagreb index is defined by ${}^mM_2(G) = \sum_{uv \in E(G)} d_u d_v$ where d_u and d_v are the degrees of vertices u and v respectively see [26]. General Randic index of G is defined as sum of $(d_u d_v)^\alpha$ over all edges

uv of G, where d_u denote the degree of vertex u of G, $R_\alpha(G)=\sum_{uv\in E(G)}(d_u d_v)^\alpha$ where α is an arbitrary real number see [27]. 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 see [8-12, 20-24,27–29]. Most recently, Munir et. Al. computed M-polynomials and related topological indices for, Bucktubes [9] and Nanostar dendrimers [28].

In the present article, we compute the closed forms of M-polynomials of single walled Titania nanotubes and represent them graphically using Mapple. As consequences, we derive some topological degree-based indices easily. We start by defining M-polynomial of a general graph, see [24]. 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 large amount of chemical experiments.

Definition If $G=(V,E)$ is a graph where V denotes vertices and E represents edges of G. Let $d_v(G)$ represents 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 $\{d_u(G),d_v(G)\}=\{i\ ,j\}$,

then M-Polynomial of graph G is defined as:

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

Topological indices are numerical parameters of graph which characterize its topology and are usually graph invariant. It describes the structure of molecules numerically. Topological indices are used in development of qualitative structure activity relationships (QSARs). Some degree-based topological indices are derived from M-polynomial [25]. Following table relates these derivations.

Topological Index	$f(x,y)$	Derivation from $M(G;x,y)$
First Zagreb	$x+y$	$(D_x+D_y)(M(G;x,y))\|_{x=y=1}$
Second Zagreb	xy	$(D_xD_y)(M(G;x,y))\|_{x=y=1}$
Second Modified Zagreb	$\frac{1}{xy}$	$(S_xS_y)(M(G;x,y))\|_{x=y=1}$

General Randić $\alpha \in \mathbb{N}$	$(xy)^{\alpha}$	$(D_x^{\alpha} D_y^{\alpha})(M(G;x,y))\|_{x=y=1}$
General Randić $\alpha \in \mathbb{N}$	$\frac{1}{(xy)^{\alpha}}$	$(S_x^{\alpha} S_y^{\alpha})(M(G;x,y))\|_{x=y=1}$
Symmetric Division Index	$\frac{x^2+y^2}{xy}$	$(D_x S_y + S_x D_y)(M(G;x,y))\|_{x=y=1}$

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

2. Main results

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

Proposition 1. Let $TNT_3[m,n]$ is the 3-layered single-walled Titania nanotube then

$$M(TNT_3[m,n],x,y) = 4mx^2y^4 + 4mx^3y^4 + 4mx^2y^6 + 2m(6n-5)x^3y^6.$$

Proof. Let $TNT_3[m,n]$ is the 3-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. Following are the tables for vertex and edge partitions of $TNT_3[m,n]$ nanotubes.

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 $TNT_3[m,n]$

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

From table 2, we see that there are four partitions, $V_{\{2\}}=\{v\grave{o}TNT_3[m,n]\,|\,d_v=2\}$,

$V_{\{3\}}=\{v\grave{o}TNT_3[m,n]\,|\,d_v=3\}$, $V_{\{4\}}=\{v\int TNT_3[m,n]\,|\,d_v=4\}$ and

$V_{\{6\}}=\{v\grave{o}TNT_3[m,n]\,|\,d_v=6\}$ for the vertex set $V(TNT_3[m,n])$ with size

$4m, 4mn-2m, 2m$ and $2mn-m$ respectively, from table 1. Now the edge set of $TNT_3[m,n]$ can be written as

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

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

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

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

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

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

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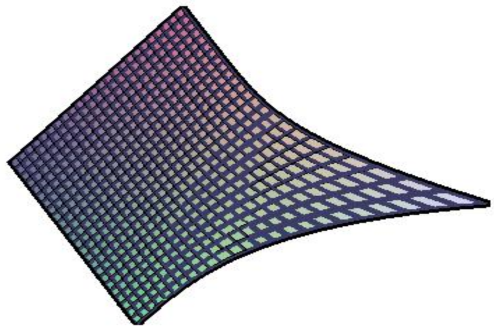

M-polynomial of 3-layered single walled titania nanotubes

Proposition 2.

Let $TNT_6[m,n]$ is the 6- layered single walled Titania nanotube then

$$M(TNT_6[m,n],x,y)=2mx^2y^2+2mx^2y^3+6mx^2y^4+8mnx^2y^5+2mx^3y^4+2m(6n-5)x^3y^5.$$

Proof.

Let $TNT_6[m,n]$ is the 6-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 3 is about the edge partitions of $TNT_6[m,n]$ and Table 4 speaks about Vertex partitions.

Table 3: 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 4: The partition of $V(G)$ of $TNT_6[m,n]$

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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

$V_{\{2\}} = \{v\grave{o}TNT_6[m,n] \mid d_v = 2\}$, $V_{\{3\}} = \{v\grave{o}TNT_6[m,n] \mid d_v = 3\}$, $V_{\{4\}} = \{v\grave{o}TNT_6[m,n] \mid d_v = 4\}$

and $V_{\{5\}} = \{v\grave{o}TNT_6[m,n] \mid d_v = 5\}$ for the vertex set $V(TNT_6[m,n])$ with size $4mn + 6m$,$4mn - 2m$,$2m$ and $4mn - 2m$ respectively, from table 4. Now the edge set of $TNT_6[m,n]$ can be written as

$$E_{\{2,2\}} = \{e = uv \in E(TNT_6[m,n]) | d_u = 2,\ d_v = 2\} \rightarrow |E_{\{2,2\}}| = 2m,$$

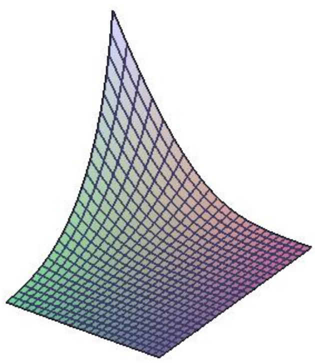
$$E_{\{2,3\}} = \{e = uv \in E(TNT_6[m,n]) | d_u = 2,\ d_v = 3\} \rightarrow |E_{\{2,3\}}| = 2m,$$

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

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

$$E_{\{3,4\}} = \{e = uv \in E(TNT_6[m,n]) | d_u = 3,\ d_v = 4\} \rightarrow |E_{\{3,4\}}| = 2m \text{ and}$$

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



M-polynomials of 6-layered single walled titania nanotubes.

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

Following important results give computation of Topological indices of 3-layered and 6-layered single-walled Titania nanotubes

Proposition 3.

Let $TNT_3[m,n]$ is the 3-layered single-walled Titania nanotube, then

1. $M_1\left(TNT_3[m,n]\right) = 108mn - 6m,$
2. $M_2(TNT_3[m,n] = 2592m^2n^2 - 288m^2n + 8m^2,$
3. ${}^mM_2(TNT_3[m,n]) = 8m^2n^2 + 8m^2n + 2m^2,$
4. $R_a(G) = (2592m^2n^2 - 288m^2n + 8m^2)^\alpha,$
5. $R_a(G) = (8m^2n^2 + 8m^2n + 2m^2)^\alpha,$
6. $SDD(G) = 360m^2n^2 + 160m^2n - 10m^2.$

Proof.

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

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

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

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

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

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

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

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

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

1. $M_1\left(TNT_3\left[m,n\right]\right)=(D_x+D_y)\left(M\left(G;x,y\right)\right)|_{x=y=1}=108mn-6m,$
2. $M_2(TNT_3[m,n])=(D_xD_y)(M(G;x,y))|_{(x=y=1)}=2592m^2n^2-288m^2n+8m^2,$
3. ${}^mM_2\left(TNT_3\left[m,n\right]\right)=(S_xS_y)\left(M\left(G;x,y\right)\right)|_{x=y=1}=8m^2n^2+8m^2n+2m^2,$
4. $R_a(G)=(D_x^\alpha D_y^\alpha)(M(G;x,y))|_{(x=y=1)}=(2592m^2n^2-288m^2n+8m^2)^\alpha,$
5. $R_a(G(S_x^\alpha S_y^\alpha)(M(G;x,y))|_{(x=y=1)}=(8m^2n^2+8m^2n+2m^2)^\alpha,\ ,$
6. $SDD(G)=(D_xS_y+S_xD_y)(M(G;x,y))|_{(x=y=1)}=360m^2n^2+160m^2n-10m^2.$

Proposition 4.

Let $TNT_6[m,n]$ is 6-layered single-walled Titania nanotube, then

1. $M_1\left(TNT_6\left[m,n\right]\right)=152mn-12m,$

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2. $M_2(TNT_6[m,n]=5200m^2n^2-816m^2n+32m^2$, ,

3. ${}^{m}M_2\left(TNT_6\left[m,n\right]\right)=32m^2n^2+\frac{68}{3}m^2n+\frac{35}{9}m^2$,

4. $R_a(G)=(5200m^2n^2-816m^2n+32m^2)^{\alpha}$,

5. $R_a(G)=(32m^2n^2+68/3m^2n+35/9m^2)^{\alpha}$,

6. $SDD\left(G\right)=1008m^2n^2+240m^2n-12m^2$.

Proof.

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

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

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

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

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

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

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

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

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

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

1. $M_1\left(TNT_3\left[m,n\right]\right)=(D_x+D_y)\left(M\left(G;x,y\right)\right)|_{x=y=1}=152mn-12m$,

2. $M_2(TNT_3[m,n])=(D_xD_y)(M(G;x,y))|_{(x=y=1)}=5200m^2n^2-816m^2n+32m^2$,

3. $^{m}M_2\left(TNT_3\left[m,n\right]\right)=(S_xS_y)\left(M\left(G;x,y\right)\right)|_{x=y=1}=32m^2n^2+\frac{68}{3}m^2n+\frac{35}{9}m^2,$

4. $R_a(G)=(D_x^{\alpha}D_y^{\alpha})(M(G;x,y))|_{(x=y=1)}=(5200m^2n^2-816m^2n+32m^2)^{\alpha},$

5. $R_a(G)=(S_x^{\alpha}S_y^{\alpha})(M(G;x,y))|_{(x=y=1)}=(32m^2n^2+68/3m^2n+35/9m^2)^{\alpha},$

6. $SDD(G)=(D_xS_y+S_xD_y)(M(G;x,y))|_{(x=y=1)}=1008m^2n^2+240m^2n-12m^2.$

3. Conclusions

In this article we computed the connectivity of Titania nanotubes through degree-based topological indices. Topological indices thus calculated for these Titania nanotubes can help us to understand the physical features, chemical reactivity, and biological activities. In this point of view, topological indices can be regarded as a score function which 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 part in determination of the significance of Single-Walled Titania Nanotubes in pharmacy [16, 17] and industry. In addition a comparison between three and six layers Titania nanotubes can be launched with the help of careful analysis of above results. The methodology described above can be extended to emerging types of neontubes: aluminosilicate/aluminugerminate [29,30,31,32].

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