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M-POLYNOMIAL OF VALENCY-BASED TOPOLOGICAL INDICES OF OPERATORS ON TITANIA NANOTUBES $T_iO_2[m, n]$ NETWORKS

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Abstract

The diagnosis of neoteric nanoparticles in the pharmaceutical and biological therapeutics area gives new directions for researchers. In this paper we discussed closed forms of valency-based topological indices of titania nanotubes. These topological indices are numerical parameter that depicts QSAR/QSPR of chemical networks requires expression for topological properties of these networks, topological indices provide those expressions of topological properties.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. A network is simply a connected graph having no multiple edges and loops. In a chemical graph the number of vertices of G adjacent to a given

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vertex u is the degree of this vertex and will be denoted by d_u. The concept of degree in graph theory is closely related (but not identical) to the concept of Valence in Chemistry, for details on the basics of graph theory, any Standard text such as [1] can be of great help.

Nano Science has attracted research interest due to its vast Applications and uses. Nanotubes, Nanocrystals and Nanowires are 3 major types of Nanomaterials. Since the discovery of the carbon nanotubes in 1991, interest in one dimensional nanomaterials has grown remarkable and a phenomenal number of research articles are being published on nanotubes as well as on nanowires.

A lot of research has been done on topological indices due to their chemical importance these indices are actually score functions that capture a variety of Physico-Chemical properties of chemical compounds such as boiling point, heat formation, heat vaporation, chromatographic retention times, surface tension, and vapor pressure.

Definition 1.1. Topological indices and Graph distance. This section emphasizes on the definitions of various topological indices of graphs. All these topological indices are distances based and $d(u, v)$ represent the length of the shortest paths between any two vertices connected with each other.

Definition 1. Harmonic index. The Harmonic index, a recently introduced topological index, is defined as follows.

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

Definition 2. The Geometric-Arithmetic Index. The Geometric-Arithmetic Index of a graph G, denoted by $GA(G)$, is defined as follows.

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u \cdot d_v}}{d_u + d_v}.$$

Definition 3. Redefined First Zagreb index. The Redefined First Zagreb Indices of a Graph G, denoted by $\operatorname{Re} ZG_1(G)$ is defined as follows.

$$\operatorname{Re} ZG_1(G) = \sum_{uv \in E(G)} \left[\frac{d_u + d_v}{d_u \cdot d_v}\right].$$

Definition 4. Redefined Second Zagreb index. The Redefined Second Zagreb Indices of a Graph G, denoted by $\operatorname{Re} ZG_2(G)$, is defined as follows.

$$\operatorname{Re} ZG_2(G) = \sum_{uv \in E(G)} \left[\frac{d_u \cdot d_v}{d_u + d_v}\right].$$

Definition 5. Redefined Third Zagreb index. The Redefined Third Zagreb Indices of a Graph G, denoted by $\operatorname{Re} ZG_3(G)$, is defined as follows.

$$\operatorname{Re} ZG_3(G) = \sum_{uv \in E(G)} d_u d_v (d_u + d_v).$$

Definition 6. Atom Bond Connectivity index. The Atom Bond Connectivity index, proposed by Ernesto Estrada et al, is defined as follows.

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \cdot d_v}}.$$

Definition 7. Augmented Zagreb Index. The Augmented Zagreb Index of a graph G, denoted by $AZI(G)$, is defined as follows.

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

Definition 8. Randic Connectivity index. The Randic Connectivity index of a graph G, denoted by $R(G)$, is defined as follows.

$$R(G) = \sum \sqrt{d_u \cdot d_v}.$$

Definition 9. Reduced Reciprocal Randic Index. The Reduced reciprocal Randic Index of a graph G, denoted by $RRR(G)$, is defined as follows.

$$RRR(G) = \sum \sqrt{(d_u - 1)(d_v - 1)}.$$

Definition 10. Banhatti Indices. The Banhatti Indices of a graph G, denoted by $B_1(G)$ and $B_2(G)$ and is defined as follows.

$$B_1(G) = \sum_{ue} [d_u + d_e]$$

$$B_2(G) = \sum_{ue} d_u \cdot d_e.$$

Where ue means that the vertex u and edge e are incident in G.

Recently several topological indices were studied, for example, in [1], [2], [3], [7], [8], [19]. In this paper, the various connectivity topological index of certain important chemical structures like Titania nanotubes are computed.

$TiO_2[m, n]$ is one of the most studied compounds in materials science. Due to outstanding properties it is used for example in photocatalysis, biomedical devices and dye-sensitized solar cells. Bulk $TiO_2[m, n]$ is a very useful environmentally friendly, non-toxic, corrosion-resistant material.

Values of the redefined first, second and third Zagreb indices for titania nanotubes $T_iO_2[m, n]$ were presented by Gao et al. [3] and the values of the Randic Index, the sum-connectivity index and the modified Randic index for titania nanotubes $T_iO_2[m, n]$ were given by Gao, Farahani and Imaran [3]. The values of incorrect results of redefined second Zagreb index and the Randic index were corrected by Tomas Vetrik [1]. In this note we were finding $S(G)$ and $R(G)$ for titania nanotubes $T_iO_2[m, n]$ for different topological indices, and also finding M-polynomial of same.

2. Results

The two-dimensional Lattice of the titania nanotube $T_iO_2[m, n]$ form $m = 4$ and $n = 6$ is presented in Figure 1. Note that m is the number of hexagons in each column and n is the number of hexagons in each row. From Figure 1 it is easy to see that n must be even (and m is any positive integer). The number of vertices in this nanotube is equal to $(m + 1)6n$ and the number of edges is $(5m + 4)2n$ [19].

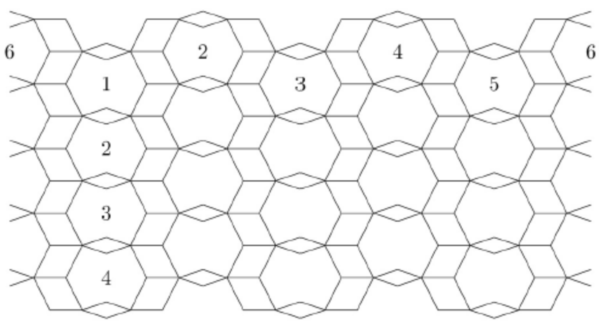

Figure 1. Titania nanotube $T_iO_2[m, n]$ for $m = 4$ and $n = 6$.

We divide the vertices of G into four sets

$$V_i = \{v \in V(TiO_2[m, n])/d_v = i\},\ i = 2, 3, 4, 5.$$

So V_i contains the vertices of degree i. Note that $V(T_iO_2[m, n]) = V_2\, U\, V_3\, U\, V_4\, U\, V_5$. From Figure 2 we get

$$|\ V_2\ | = (m + 2)2n,\ |\ V_3\ | = 2mn,\ |\ V_4\ | = 2n,\ |\ V_5\ | = 2mn.$$

Let $E_{ij} = \{uv \in E(G)d_u = i,\ d_v = j\}$.

This means that the set E_{ij} contains the edges incident with one vertex of degree i and the other vertex of degree j.

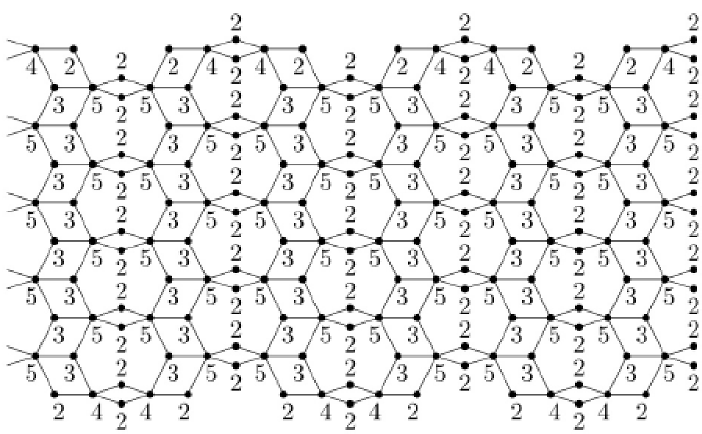

Figure 2. Titania nanotube $T_iO_2[m, n]$ with degree assigned to the vertices.

In Figure 2 we can see the degree of every vertex, thus we can easily get

$$| E_{5,3} | = (3m - 1)2n, \; | E_{5,2} | = (2m + 1)2n, \; | E_{4,3} | = 2n, \; | E_{4,2} | = 6n.$$

We have $E(T_iO_2[m, n]) = E_{5,3}UE_{5,2}UE_{4,3}UE_{4,2}$.

3. Subdivision Graph

The subdivision graph $S(G)$ is the graph obtained from G by replacing each of its edge by a path of length 2, or equivalently by inserting an additional vertex into each edge of G. The p-subdivision graph $S(G)$ is the graph obtained from G by inserting each of its edge by a path of length $p + 1$, or equivalent by inserting p additional vertices into each edge of G. The number of vertices in this subdivision nanotube is equal to $2n(8m + 7)$ and the number of edges is $4n(5m + 7)$.

Let $E_{i,j} = \{uv \in E(G)d_u = i, d_v = j\}$

$$| E_{2,2} | = 4n(m + 2), \; | E_{2,3} | = 6mn, \; | E_{2,4} | = 8n, \; | E_{2,5} | = 10mn.$$

Theorem 3.1. *The harmonic index of subdivision titania nanotubes* $T_iO_2[m, n]$ *is*

$$H[S(T_iO_2[m, n])] = 2n\left[\frac{127}{35}m + \frac{10}{3}\right].$$

Proof. Since $E(T_iO_2[m, n]) = E_{2,2}UE_{2,3}UE_{2,4}UE_{2,5}$ for harmonic index of subdivision titania nanotubes we have

$$H[S(T_iO_2[m, n])] = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$$

$$= 4n(m + 2) \cdot \left(\frac{2}{2 + 2}\right) + 6mn \cdot \left(\frac{2}{2 + 3}\right) + 8n \cdot \left(\frac{2}{2 + 4}\right)$$

$$+ 10mn \cdot \left(\frac{2}{2 + 5}\right)$$

$$= 2n(m+2) + \frac{12}{5}mn + \frac{8}{3n} + \frac{20}{7}mn$$

$$= 2mn + 4n + \frac{12}{5}mn + \frac{8}{3}n + \frac{20}{7}mn$$

$$= \frac{254}{35}mn + \frac{20}{3}n$$

$$= 2n\left[\frac{127}{35}mn + \frac{10}{3}\right].$$

Theorem 3.2. *The Geometric-Arithmetic index, The Redefined First Zagreb index, The Redefined Second Zagreb index, The Redefined Third Zagreb index, The Augmented Zagreb index, The Randic Connectivity index, The Reduced reciprocal Randic index, Banhatti indices of Subdivision Titania nanotubes* $T_iO_2[m, n]$ *is*

(1) $GA[S(T_iO_2[m, n])] = \left[4 + \frac{12\sqrt{6}}{5} + \frac{20\sqrt{10}}{7}\right]mn + \left[8 + \frac{16\sqrt{2}}{3}\right]n.$

(2) $\text{Re}\, Z_1[S(T_iO_2[m, n])] = 2n[8m + 7].$

(3) $\text{Re}\, Z_2[S(T_iO_2[m, n])] = n\left[\frac{892}{35}m + \frac{56}{3}\right].$

(4) $\text{Re}\, Z_3[S(T_iO_2[m, n])] = 8n[93m + 64].$

(5) $ABC[S(T_iO_2[m, n])] = \frac{4n}{\sqrt{2}}[5m + 4].$

(6) $AZI[S(T_iO_2[m, n])] = 32n[5m + 4] = 8\sqrt{2}ABC[S(T_iO_2[m, n])].$

(7) $R[S(T_iO_2[m, n])] = [4 + 3\sqrt{6} + 5\sqrt{10}]2mn + [1 + \sqrt{2}]16n.$

(8) $RRR[S(T_iO_2[m, n])] = [4 + \sqrt{2}]6mn + [1 + \sqrt{3}]8n.$

(9) $B_1[S(T_iO_2[m, n])] = 4n[67m + 44].$

(10) $B_2[S(T_iO_2[m, n])] = 8n[59m + 32].$

Proof. We leave the proof for the reader.

4. Graph Operators

The operator $R(G)$ [17] is the graph obtained from G by adding a new vertex corresponding to each edge of G and by joining each new vertex to the end vertices of the edge corresponding to it.

The number of vertices in this subdivision nanotube is equal to $2n(8m+7)$ and the number of edges is $6n(5m+4)$.

Let $E_{i,j} = \{uv \in E(G) d_u = i, d_v = j\}$.

This means that the set $E_{i,j}$ contains the edges incident with one vertex of degree i and the other vertex of degree j. In Figure 2 we can see the degree of every vertex, thus we can easily get.

$$|E_{2,4}| = (m+2)4n, |E_{2,6}| = 6mn, |E_{2,8}| = 8n, |E_{2,10}| = 10mn,$$

$$|E_{4,8}| = 6n, |E_{4,10}| = (2m+1)2n, |E_{6,8}| = 2n, |E_{6,10}| = (3m-1)2n.$$

Theorem 4.1. *The Harmonic index of semi total point graph* $R(G)$ *of Titania nanotubes* $T_iO_2[m, n]$ *is,* $H[R(T_iO_2[m, n])] = n\left[\frac{97}{28}m + \frac{475}{84}\right]$.

Proof. Since $E(T_iO_2[m, n]) = E_{2,4}UE_{2,6}UE_{2,8}UE_{2,10}UE_{4,8}UE_{4,10}UE_{6,8}UE_{6,10}$ for Harmonic index of semi total point graph $R(G)$ of titania nanotubes.

We have,

$$H[S(T_iO_2[m, n])] = \sum_{uv \in E(G)} \frac{2}{d_u + d_v} = 4n(m+2)\left(\frac{2}{2+4}\right) + 6mn \cdot \left(\frac{2}{2+6}\right)$$

$$+ 8n \cdot \left(\frac{2}{2+8}\right) + 10mn \cdot \left(\frac{2}{2+10}\right) + 6n \cdot \left(\frac{2}{4+8}\right)$$

$$+ 2n(2m+1) \cdot \left(\frac{2}{4+10}\right) + 2n \cdot \left(\frac{2}{6+8}\right) + 2n(3m-1) \cdot \left(\frac{2}{6+10}\right)$$

$$= \frac{97}{28}mn + \frac{475}{84}n$$

$$= n\left[\frac{97}{28}m + \frac{475}{84}\right].$$

Theorem 4.2. *The Geometric-Arithmetic index, The Redefined First Zagreb index, The Redefined Second Zagreb index, The Redefined Third Zagreb index, The Augmented Zagreb index, The Randic Connectivity index, The Reduced reciprocal Randic index, Banhatti indices of semi total point graph* $R(G)$ *of Titania nanotubes* $T_iO_2[m, n]$ *is*

(1) $GA[R(T_iO_2[m, n])] = \left[2\sqrt{2} + 3\sqrt{3} + \frac{10}{3} + 3\frac{\sqrt{15}}{2} + 8\frac{\sqrt{10}}{7}\right]mn$

$$+ \left[8\sqrt{2} - \frac{\sqrt{15}}{2} + \frac{32}{5} + \frac{4\sqrt{10}}{7} + \frac{8\sqrt{3}}{7}\right]n.$$

(2) $\operatorname{Re} Z_1[R(T_iO_2[m, n])] = \left[13 + \frac{14}{10} + \frac{24}{15}\right]mn + \left[11 + \frac{9}{4} + \frac{7}{10} + \frac{7}{12} - \frac{8}{12}\right]n.$

(3) $\operatorname{Re} Z_2[R(T_iO_2[m, n])] = \left[\frac{1381}{21} + \frac{4414}{105}\right]n.$

(4) $\operatorname{Re} Z_3[R(T_iO_2[m, n])] = [11168m + 4672]n.$

(5) $ABC[R(T_iO_2[m, n])] = \left[10\sqrt{2} + \frac{4\sqrt{3}}{\sqrt{10}} + \frac{6\sqrt{7}}{\sqrt{10}}\right]mn$

$$+ \left[9\sqrt{2} + \frac{3\sqrt{5}}{2} + \frac{2\sqrt{3}}{10} - \frac{2\sqrt{7}}{10}\right]n.$$

(6) $AZI[R(T_iO_2[m, n])] = \left[160 + \frac{4000}{27} + 6\left(\frac{30}{7}\right)^3\right]mn$

$$+ \left[256 + \frac{24576}{125} + \frac{2000}{27} - 2\left(\frac{30}{7}\right)^3\right]n.$$

(7) $R[R(T_iO_2[m, n])] = [8\sqrt{2} + 12\sqrt{3} + 20\sqrt{5} + 8\sqrt{10} + 12\sqrt{15}]mn + [32 + 40\sqrt{2}$ $+ 8\sqrt{3} + 4\sqrt{10} - 4\sqrt{15}]n.$

(8) $RRR[R(T_iO_2[m, n])] = [16\sqrt{3} + 24\sqrt{5} + 30]mn + [14\sqrt{3} - 6\sqrt{5} + 8\sqrt{7}$

$+ 6\sqrt{21} + 2\sqrt{35}]n.$

(9) $B_1[R(T_iO_2[m, n])] = 96n[10m + 7].$

(10) $B_2[R(T_iO_2[m, n])] = 48n[75m + 37].$

Proof. We leave the proof for the reader.

5. *M*-Polynomial

Let G be a simple connected graph. The M-Polynomial [4] of G is defined as

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

Where $\delta = Min\{d_v | v \in V(G)\}$, $\Delta = Max\{d_v | v \in V(G)\}$, and $m_{i,j}(G)$ is the number of edges $uv \in E(G)$ such that $\{d_u, d_v\} = \{i, j\}$.

Let G be the simple connected graph. The first Zagreb index is defined as

$$M_1(G) = \sum_{u \in V(G)} (d_v)^2$$

and the second Zagreb index is defined as

$$M_2(G) = \sum_{u \in V(G)} d_u d_v.$$

The Second modified Zagreb index is defined as

$$^m M_2(G) = \sum_{u \in E(G)} \frac{1}{d_u d_v}.$$

The following Table 1 relates some degree-based topological indices from M-polynomial. [12, 13, 14, 15]

Table 1. Derivation of some degree-based topological indices from *M*-Polynomial.

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	$(D_x D_y)(M(G; x, y))\|x = y = 1$
Second Modified Zagreb	$\frac{1}{xy}$	$(S_x S_y)(M(G; x, y))\|x = y = 1$
General Randic $\alpha \in N$	$(xy)^{\alpha}$	$(D_x^{\alpha} \cdot D_y^{\alpha})(M(G; x, y))\|x = y = 1$
General Randic $\alpha \in N$	$\frac{1}{xy}^{\alpha}$	$(S_x^{\alpha} \cdot S_y^{\alpha})(M(G; x, y))\|x = y = 1$
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

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

$$S_y = \int_0^y \frac{f(x, y)}{t} dt.$$

In this section, we provide our main computational results. We divide this section into three subsections.

The Titania nanotube $T_i O_2[m, n]$ form $m = 4, n = 6,$ where m is the number of hexagons in each column and n is the number of hexagons in each row. Figure 1 illustrates this. In the following Theorem, we compute the *M*-polynomial for titania nanotube.

Theorem 5.1. *Let* $T_i O_2[m, n]$ *be the structure of titania nanotube. Then*

$$M(T_i O_2[m, n]; x, y) = 2n(2m + 3)x^2 y^4 + 2nx^2 y^5 + 2nx^3 y^4 + 2n(3m - 1)x^3 y^5.$$

Proof. From the 2-Dimensional lattice of $T_i O_2[m, n],$ we can see that there are four partitions of vertices.

$$| V_2 | = (m+2)2n, \; | V_3 | = 2mn, \; | V_4 | = 2n, \; | V_5 | = 2mn$$

the edge set of $T_i O_2[m, n]$ can be partitioned as $| E_{2,4} | = 6n$, $| E_{3,4} | = 2n$, $| E_{2,5} | = (2m+1)2n$, $| E_{3,5} | = (3m-1)2n$.

thus, the M-Polynomial of $T_i O_2[m, n]$ is

$$M(T_i O_2[m, n]; x, y) = \sum_{i \le j} m_{i,j}(T_i O_2[m, n]) x^i y^i$$

$$= 2n(2m+3)x^2 y^4 + 2nx^2 y^5 + 2nx^3 y^4 + 2n(3m-1)x^3 y^5$$

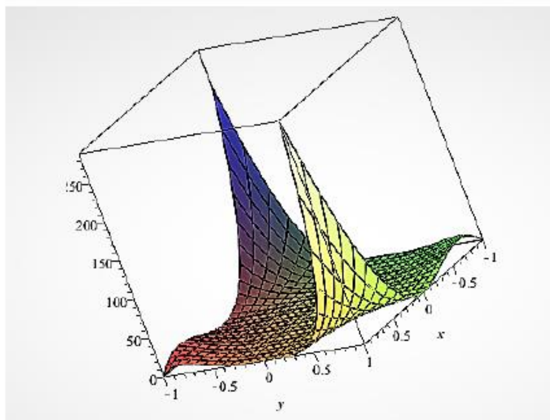

Figure 3 is a graph for the M-polynomial of $T_i O_2[m, n]$ titania nanotube.

Theorem 5.2. *Let* $T_i O_2[m, n]$ *be the structure of titania nanotube, then*

$$M_1(T_i O_2[m, n]) = 24n[3m+2]$$

$$M_2(T_i O_2[m, n]) = 2n[61m+31]$$

$$^m M_2(T_i O_2[m, n]) = n\left[\frac{9}{10}m + \frac{37}{30}\right]$$

$$SDD(T_i O_2[m, n]) = n\left[\frac{118}{5}m + \frac{613}{30}\right].$$

Proof. We leave the proof for the reader.

Theorem 5.3. *Let* $S(T_iO_2[m, n])$ *be the structure of subdivision of titania nanotube, then*

$$M[S(T_iO_2[m, n]); x, y] = 4n(m+2)x^2y^2 + 6mnx^2y^3 + 8nx^2y^4 + 10mnx^2y^5.$$

Proof. We leave the proof for the reader.

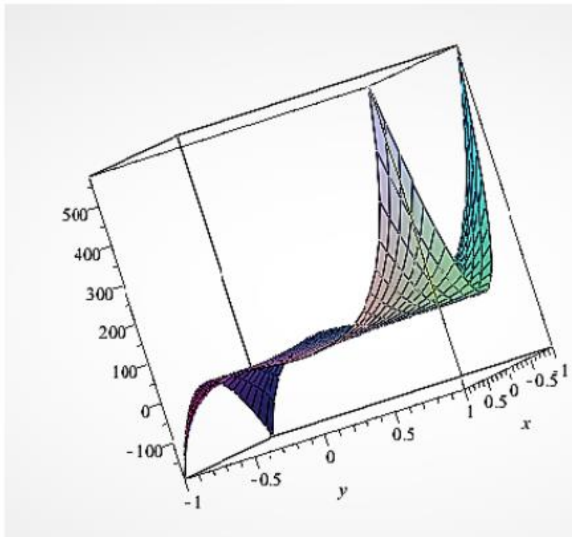

Figure 4. *M*-Polynomial of subdivision of titania nanotube.

Theorem 5.4. *Let* $S(T_iO_2[m, n])$ *be the structure of subdivision of titania nanotube, then*

$$M_1[S(T_iO_2[m, n])] = 4n[29m + 20]$$

$$M_2[S(T_iO_2[m, n])] = 8n[19m + 12]$$

$$^mM_2[S(T_iO_2[m, n])] = 3n[m + 1]$$

$$SDD[S(T_iO_2[m, n])] = 2n[25m + 18].$$

Proof. We leave the proof for the reader.

Theorem 5.5. *Let* $R(T_iO_2[m, n])$ *be the structure of semi total point graph of Titania nanotube, then*

$$M[R(T_iO_2[m, n]); x, y] = 4n(m+2)x^2y^4 + 6mnx^2y^6 + 8nx^2y^8 + 10mnx^2y^{10}$$
$$+ 6nx^4y^8 + 2n(2m+1)x^4y^{10} + 2nx^6y^8 + 2n(3m-1)x^6y^{10}.$$

Proof. We leave the proof for the reader.

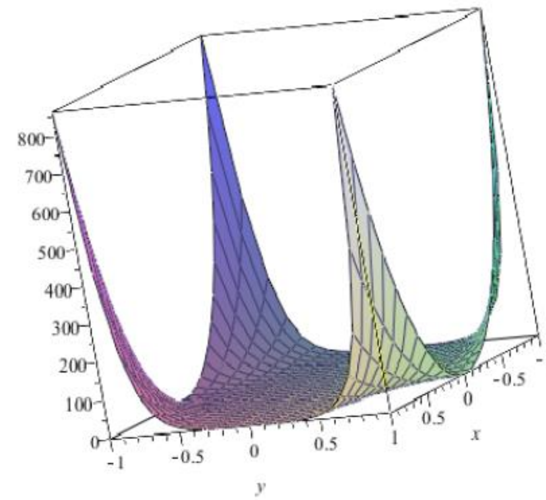

Figure 5. M-Polynomial of $R(T_iO_2 - 2[m, n])$ of titania nanotube.

Theorem 5.6. *Let* $R(T_iO_2[m, n])$ *be the structure of semi total point graph of Titania Nanotube*, *then*

$$M_1[R(T_iO_2[m, n])] = 8n[43m + 34]$$

$$M_2[R(T_iO_2[m, n])] = 8n[103m + 55]$$

$$^mM_2[R(T_iO_2[m, n])] = n\left[\frac{17}{10}m + \frac{431}{240}\right]$$

$$SDD[R(T_iO_2[m, n])] = \frac{n}{5}\left[536m + \frac{1487}{4}\right].$$

Proof. We leave the proof for the reader.

6. Conclusions

In this article, to conclude with we sketch the surfaces co-ordinated to M-polynomial and characterize few parts about these Titania nanotubes.

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