Sigma J Eng & Nat Sci 35 (4), 2017, 707-714

Sigma Journal of Engineering and Natural Sciences
Sigma Mühendislik ve Fen Bilimleri Dergisi

Research Article

COMPUTING HYPER ZAGREB INDEX AND M-POLYNOMIALS OF TITANIA NANOTUBES $TiO_2[m,n]$

Mehdi REZAEI[1], Wei GAO[2], Muhammad K SIDDIQUI[3], Mohammad R. FARAHANI*[4]

[1]*Department of Mathematics, Buein Zahra Technical University, Buein Zahra, Qazvin-IRAN;* ORCID:0000-0001-6999-9703
[2]*School of Information and Technology, Yunnan Normal University, Kunming-CHINA;* ORCID:0000-0001-8744-9334
[3]*Department of Mathematics, Comsats Institute of Information Technology, Sahiwal-PAKISTAN;* ORCID:0000-0002-2607-4847
[4]*Department of Applied Mathematics, Iran University of Science and Technology (IUST), Narmak, Tehran-IRAN;* ORCID:0000-0003-2926-4280

Received: 01.03.2017 Revised: 08.09.2017 Accepted: 22.09.2017

ABSTRACT

The concept of hyper Zagreb index, Zagreb and M-polynomials are establish in chemical graph theory based on the degree of the vertex. It is reported that these indices are useful in the study of anti-inflammatory activities of certain chemical networks. In this paper, we determine hyper Zagreb index, Zagreb and M-polynomials for an infinite class of Titania nanotubes $TiO_2[m,n]$.

Keywords: Hyper Zagreb index, Zagreb polynomials, M-polynomial, TiO_2 nanotubes.

1. INTRODUCTION

In the last decade, graph theory has been found a considerable use in this area of research. Graph theory has provided chemist with a variety of useful tools, such as topological indices. Chem-informatics is new subject which is a combination of chemistry, mathematics and information science. It studies Quantitative structure-activity (QSAR) and structure-property (QSPR) relationships that are used to predict the biological activities and properties of chemical compounds. In the QSAR /QSPR study, physico-chemical properties and topological indices such as hyper Zagreb index, first multiple Zagreb index, second multiple Zagreb index and Zagreb polynomials are used to predict bioactivity of the chemical compounds.

More preciously chemical graph theory is a branch of mathematical chemistry in which we apply tools from graph theory to model the chemical phenomenon mathematically. This theory plays a prominent role in the fields of chemical sciences.

* Corresponding Author: e-mail: mrfarahani88@gmail.com, tel: +98 919 2478265

A molecular graph is a simple graph in which the vertices denote atoms and the edges represent chemical bonds between these atoms. The hydrogen atoms are often omitted in a molecular graph. Let G be a molecular graph with vertex set $V(G)=\{a_1,a_2,\ldots,a_n\}$ and edge set $E(G)$. We denote the order and size of G by $|V(G)|$ and $|E(G)|$, respectively. An edge in $E(G)$ with end vertices a and b is denoted by ab. Two vertices a and b are said to be adjacent if there is an edge between them. The set of all vertices adjacent to a vertex a is said to be the neighbourhood of a, denoted as $N(a)$. The number of vertices in $N(a)$ is said to be the degree of a, denoted by $d(a)$. The maximum and minimum vertex degrees in a graph G, respectively denoted by $\Delta(G)$ and $\delta(G)$, are defined as $\max\{d(a)\mid a\in V(G)\}$ and $\min\{d(a)\mid a\in V(G)\}$, respectively. A (a_1,a_n)-path on n vertices is denoted by P_n and is defined as a graph with vertex set $\{a_i:1\le i\le n\}$ and edge set a_ia_{i+1}, for $1\le i\le n-1$. The length of a path P_n is the number of edges in it, that is, $n-1$.

A topological index is a numeric quantity associated with a graph which characterizes the topology of graph and is invariant under graph automorphism. There are some major classes of topological indices such as distance based topological indices, degree based topological indices and counting related polynomials and indices of graphs. Among these classes degree based topological indices are of great importance and play a vital role in chemical graph theory and particularly in chemistry. In more precise way, a topological index Top(G) of a graph G, is a number with the property that for every graph H isomorphic to G, Top(H)=Top(G). The concept of topological index came from work done by Wiener [1]. while he was working on boiling point of paraffin. He named this index as path number. Later on, the path number was renamed as Wiener index. The Wiener index is the first and most studied topological index, both from theoretical point of view and applications, and defined as the sum of distances between all pairs of vertices in G, see for details [2].

One of the oldest topological index is the first and second Zagreb index an introduced by I. Gutman and N. Trinajstić [3] on based degree of vertices of G in 1972 and are defined as:

$$M_1(G)=\sum_{uv\in E(G)}\left[d(u)+d(v)\right],\ M_2(G)=\sum_{uv\in E(G)}\left[d(u)\times d(v)\right]$$

M. Ghorbani and N. Azimi [4] define two new versions of Zagreb indices of a graph G in 2012. The first multiple Zagreb index $PM_1(G)$, second multiple Zagreb index $M_2(G)$ and these indices are defined as:

$$PM_1(G)=\prod_{uv\in E(G)}\left[d(u)+d(v)\right],\ PM_2(G)=\prod_{uv\in E(G)}\left[d(u)\times d(v)\right]$$

In 2013, G.H. Shirdel, H. RezaPour and A.M. Sayadi [5] introduced a new degree based of Zagreb index named 'hyper Zagreb index' as

$$HM(G)=\sum_{uv\in E(G)}\left[d(u)+d(v)\right]^2 \tag{1}$$

In 2004, I. Gutman and K.C. Das [6] define the first and second Zagreb Polynomial in the following way.:

$$M_1(G,x)=\sum_{uv\in E(G)}x^{[d(u)+d(v)]} \tag{2}$$

$$M_2(G,x) = \sum_{uv \in E(G)} x^{[d(u) \times d(v)]} \tag{3}$$

The properties of $M_1(G,x)$, $M_2(G,x)$ polynomials for s ome chemical structures have been studied in the literature [6-10].

In 2015, E. Deutshi and S. Klavžar [11] define a new polynomial namely 'M-polynomial' based on the degree of the vertex in the following way:

$$M_1(G,x,y) = \sum_{uv \in E(G)} x^{[d(u)]} y^{[d(v)]} \tag{4}$$

Motivated by the idea of E. Deutshi and S. Klavžar [11], we define the multiplicative version of 'M- polynomial' in the following way.

$$M_2(G,x,y) = \prod_{uv \in E(G)} x^{[d(u)]} y^{[d(v)]} \tag{5}$$

Nowadays there is an extensive research activity on HM(G), $PM_1(G)$, M_2 (G) indices and $M_1(G,x)$, $M_1(G,x)$, M(G,xy), $M_1(G,x,y)$ and their variants, For further study of topological indices of various graph families, see [12-20].

2. TITANIA NANOTUBE $TiO_2[m,n]$

Titania nanotubes comprehensively study in materials science. Titania nanotubes were systematically synthesized during the last 10-15 years using different methods and carefully studied as prospective technological materials. Since the growth mechanism for TiO_2 nanotubes is still not well defined, their comprehensive theoretical studies attract enhanced attention. The TiO_2 sheets with a thickness of a few atomic layers were found to be remarkably stable [21-36].

The graph of the Titania nanotube $TiO_2[m,n]$ is presented in Figure 1, where m denotes the number of octagons in a column and n denotes the number of octagons in a row of the Titania nanotube.

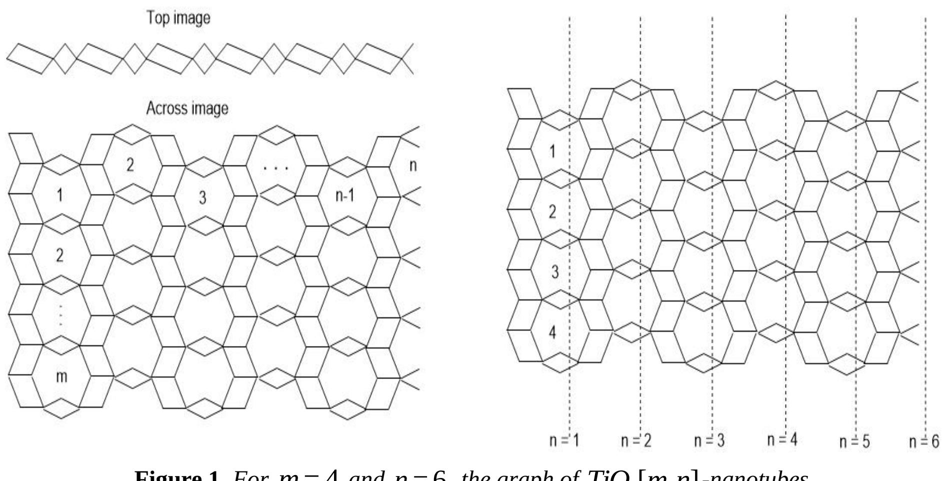

Figure 1. *For $m = 4$ and $n = 6$, the graph of $TiO_2[m,n]$-nanotubes*

M.A. Malik and M. Imran [37] compute the first and second Zagreb index, first and second multiple Zagreb index for an infinite class of Titania nanotubes $TiO_2[m,n]$. In the next Theorems we compute hyper Zagreb index, Zagreb and M- polynomials for an infinite class of Titania nanotubes $TiO_2[m,n]$.

For this we perform some necessary calculations for computing the hyper Zagreb index, Zagreb and M-polynomials defined in the previous section.

Let us define the partitions for the vertex set and edge set of the Titania nanotube TiO_2, for $\delta(G) \le k \le \Delta(G)$, $2\delta(G) \le i \le 2\Delta(G)$ and $\delta(G)^2 \le j \le \Delta(G)^2$, then we have

$$V_k = \{v \in V(G) \,|\, d(v) = k\},$$
$$E_i = \{e = uv \in E(G) \,|\, d(u) + d(v) = i\},$$
$$E_j^* = \{e = uv \in E(G) \,|\, d(u)d(v) = j\}.$$

In the molecular graph of TiO_2 nanotubes, we can see that $2 \le d(v) \le 5$. So, we have the vertex partitions as follows.

$$V_2 = \{u \in V(G) \,|\, d(u) = 2\},$$
$$V_3 = \{u \in V(G) \,|\, d(u) = 3\},$$
$$V_4 = \{u \in V(G) \,|\, d(u) = 4\},$$
$$V_5 = \{u \in V(G) \,|\, d(u) = 5\}.$$

Similarly, the edge partitions of the graph of TiO_2 nanotubes are as follows.

$$E_6 = E_8^* = \{e = uv \in E(G) \,|\, d(u) = 2 \,\&\, d(v) = 4\},$$
$$E_7 = E_{10}^* \cup E_{12}^* = \{e = uv \in E(G) \,|\, d(u) = 2 \,\&\, d(v) = 5\}$$
$$\cup \{e = uv \in E(G) \,|\, d(u) = 3 \,\&\, d(v) = 4\},$$
$$E_8 = E_{15}^* = \{e = uv \in E(G) \,|\, d(u) = 3 \,\&\, d(v) = 5\}.$$

Since for every vertex $v \in V(G)$, $d(v)$ belongs to exactly one class V_k for $2 \le k \le 5$ and for every edge $uv \in E(G)$, $d(u) + d(v)$ (resp. $d(u)d(v)$) belongs to exactly one class E_i (resp. E_j^*) for $2\delta(G) \le i \le 2\Delta(G)$ and $\delta(G)^2 \le j \le \Delta(G)^2$. So, the vertex partitions V_k and the edge partitions E_i and E_j^* are collectively exhaustive, that is

$$\bigcup_{k=\delta(G)}^{\Delta(G)} V_k = V(G), \quad \bigcup_{i=2\delta(G)}^{2\Delta(G)} E_i = E(G), \quad \bigcup_{j=\delta^2(G)}^{\Delta^2(G)} E_j^* = E(G).$$

When $m=1$, the number of vertices of degree 2 in $TiO_2[1,n]$ are $2n + n + 1 \times (2n) + n$. Thus for $TiO_2[m,n]$, we have $|V_2| = 2n + n + m(2n) + n = 2mn + 4n$. Similarly, the cardinalities of all the vertex and edge partitions can be obtained, which are presented in Table 1.

Table 1. The vertex partitions of the TiO_2 nanotubes along with their cardinalities.

Vertex partition	V_2	V_3	V_4	V_5
Cardinality	$2mn+4n$	$2mn$	$2n$	$2mn$

Table 2. The edge partitions of the TiO_2 nanotubes along with their cardinalities.

Vertex partition	$E_6 = E_8^*$	E_7	$E_8 = E_{15}^*$	E_{10}^*	E_{12}^*
Cardinality	$6n$	$4mn+4n$	$6mn-2n$	$4mn+2n$	$2n$

Now we compute hyper Zagreb index, Zagreb polynomials and M-polynomials in the following theorems.

Theorem 1. *The hyper Zagreb index of the* TiO_2 *nanotube is given by*

$$HM(TiO_2) = 284n + 580mn.$$

Proof. From equation (1) and using cardinalities of the edge partitions from Table 2, we get,

$$\begin{aligned} HM(TiO_2) &= \sum_{uv\in E(G)} \left[d(u)+d(v)\right]^2 \\ &= \sum_{uv\in E_6(TiO_2)} \left[d(u)+d(v)\right]^2 + \sum_{uv\in E_7(TiO_2)} \left[d(u)+d(v)\right]^2 + \sum_{uv\in E_8(TiO_2)} \left[d(u)+d(v)\right]^2 \\ &= 36\left(\left|E_6(TiO_2)\right|\right) + 49\left(\left|E_7(TiO_2)\right|\right) + 64\left(\left|E_8(TiO_2)\right|\right) \\ &= 36\left(6n\right) + 49\left(4mn+4n\right) + 64\left(6mn-2n\right) \\ &= 284n + 580mn. \end{aligned}$$

Theorem 2. *The first Zagreb polynomial of the* TiO_2 *nanotube is given by*

$$M_1(TiO_2, x) = \left(6n\right)x^6 + \left(4mn+4n\right)x^7 + \left(6mn-2n\right)x^8.$$

Proof. From equation (2) and using cardinalities of the edge partitions from Table 2, we get,

$$\begin{aligned} M_1(TiO_2, x) &= \sum_{uv\in E(TiO_2)} x^{\left[d(u)+d(v)\right]} \\ &= \sum_{uv\in E_6(TiO_2)} x^{\left[d(u)+d(v)\right]} + \sum_{uv\in E_7(TiO_2)} x^{\left[d(u)+d(v)\right]} + \sum_{uv\in E_8(TiO_2)} x^{\left[d(u)+d(v)\right]} \\ &= \left(\left|E_6(TiO_2)\right|\right)x^6 + \left(\left|E_7(TiO_2)\right|\right)x^7 + \left(\left|E_8(TiO_2)\right|\right)x^8 \\ &= \left(6n\right)x^6 + \left(4mn+4n\right)x^7 + \left(6mn-2n\right)x^8 . \end{aligned}$$

Theorem 3. *The second Zagreb polynomial of the* TiO_2 *nanotube is given by*

$$M_2(TiO_2, x) = \left(6n\right)x^8 + \left(4mn+4n\right)x^{10} + \left(6mn-2n\right)x^{15}.$$

Proof. From equation (3) and using cardinalities of the edge partitions from Table 2, we get,

$$
\begin{aligned}
M_2(TiO_2, x) &= \sum_{uv\in E(TiO_2)} x^{[d(u)\times d(v)]} \\
&= \sum_{uv\in E_6(TiO_2)} x^{[d(u)\times d(v)]} + \sum_{uv\in E_7(TiO_2)} x^{[d(u)\times d(v)]} + \sum_{uv\in E_8(TiO_2)} x^{[d(u)\times d(v)]} \\
&= \left(\left|E_6(TiO_2)\right|\right)x^8 + \left(\left|E_7(TiO_2)\right|\right)x^{10} + \left(\left|E_8(TiO_2)\right|\right)x^{15} \\
&= \left(6n\right)x^8 + \left(4mn+4n\right)x^{10} + \left(6mn-2n\right)x^{15}.
\end{aligned}
$$

Theorem 4. *The first M- polynomial of the TiO_2 nanotube is given by*

$$M_1(TiO_2, x, y) = \left(6n\right)x^2y^4 + \left(4mn+4n\right)x^2y^5 + \left(6mn-2n\right)x^3y^5.$$

Proof. From equation (4) and using cardinalities of the edge partitions from Table 2, we get,

$$
\begin{aligned}
M_1(TiO_2, x, y) &= \sum_{uv\in E(TiO_2)} x^{[d(u)]}y^{[d(v)]} \\
&= \sum_{uv\in E_6(TiO_2)} x^{[d(u)]}y^{[d(v)]} + \sum_{uv\in E_7(TiO_2)} x^{[d(u)]}y^{[d(v)]} + \sum_{uv\in E_8(TiO_2)} x^{[d(u)]}y^{[d(v)]} \\
&= \left(\left|E_6(TiO_2)\right|\right)x^2y^4 + \left(\left|E_7(TiO_2)\right|\right)x^2y^5 + \left(\left|E_8(TiO_2)\right|\right)x^3y^5 \\
&= \left(6n\right)x^2y^4 + \left(4mn+4n\right)x^2y^5 + \left(6mn-2n\right)x^3y^5.
\end{aligned}
$$

Theorem 5. *The second M- polynomial of the TiO_2 nanotube is given by*

$$M_2(TiO_2, x, y) = x^{26mn+16n}y^{50mn+32n}$$

Proof. From equation (5) and using cardinalities of the edge partitions from Table 2, we get,

$$
\begin{aligned}
M_2(TiO_2, x, y) &= \prod_{uv\in E(TiO_2)} x^{[d(u)]}y^{[d(v)]} \\
&= \prod_{uv\in E_8^*(TiO_2)} x^{d(u)}y^{d(v)} \times \prod_{uv\in E_{10}^*(TiO_2)} x^{d(u)}y^{d(v)} \times \prod_{uv\in E_{12}^*(TiO_2)} x^{d(u)}y^{d(v)} \times \prod_{uv\in E_{15}^*(TiO_2)} x^{d(u)}y^{d(v)} \\
&= \left(x^2y^4\right)^{\left(\left|E_8^*(TiO_2)\right|\right)} \times \left(x^2y^5\right)^{\left(\left|E_{10}^*(TiO_2)\right|\right)} \times \left(x^3y^4\right)^{\left(\left|E_{12}^*(TiO_2)\right|\right)} \times \left(x^3y^5\right)^{\left(\left|E_{15}^*(TiO_2)\right|\right)} \\
&= \left(x^2y^4\right)^{(6n)} \times \left(x^2y^5\right)^{(4mn+2n)} \times \left(x^3y^4\right)^{(2n)} \times \left(x^3y^5\right)^{(6mn-2n)} \\
&= \left(x^{12n}y^{24n}\right)\left(x^{2(4mn+2n)}y^{5(4mn+2n)}\right)\left(x^{6n}y^{8n}\right)\left(x^{3(6mn-2n)}y^{5(6mn-2n)}\right) \\
&= x^{26mn+16n}y^{50mn+32n}.
\end{aligned}
$$

3. CONCLUSION

Since Topological indices have also been used as branching indices and have found applications in QSPR and QSAR studies. In this paper, we have deal with Titania nanotubes and studied their topological indices. More preciously, we determine hyper Zagreb index, Zagreb and M-polynomials for an infinite class of Titania nanotubes $TiO_2[m,n]$. In the future, we are interested to design some new architectures/networks and then study their topological indices which will be quite helpful to understand their underlying topologies.

REFERENCES

[1] Wiener H., (1947) Structural Determination of Paraffin Boiling Points, *Journal of the American Chemical Society*, 69(1), 17-20.

[2] Dobrynin A.A., Entringer R. and Gutman I., (2001) Wiener Index of Trees: Theory and Applications, *Acta Applicandae Mathematica*, 66(3), 211–249.

[3] Gutman I. and Trinajstic N., (1972) Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons, *Chemical Physics Letters*, 17(4), 535-538.

[4] Ghorbani M. and Azimi N., (2012) Note on multiple Zagreb indices, *Iranian Journal of Mathematical Chemistry*, 3(2), 137-143.

[5] Shirdel G.H., RezaPour H. and Sayadi A. M., (2013) The Hyper-Zagreb Index of Graph Operations, *Iranian Journal of Mathematical Chemistry*, 4(2), 213-220.

[6] Gutman I. and Das K. C., (2004) The First Zagreb Index 30 Years After, *MATCH Communications in Mathematical and in Computer Chemistry*, 50, 83–92.

[7] Nikolic S., Kovacevic G., Miliccevic, A., Trinajstic, N., (2003) The Zagreb indices 30 years after. *Croat. Chem. Acta* , 76, 113-124.

[8] Wang S., Wei B., (2015) Multiplicative Zagreb indices of k-trees, *Discrete Applied Mathematics* 180, 168-175.

[9] Wang S., Wei B., (2016) Multiplicative Zagreb indices of Cacti, *Discrete Mathematics, Algorithms and Applications,* 8(3), 1650040.

[10] Li X., Shi Y., (2008) A survey on the Randic index, *MATCH Commun. Math. Comput. Chem.* 59(1), 127-156.

[11] Deutschi E. and Klavžar S., (2015) M-polynomial and degree-based topological indices, *Iranian Journal of Mathematical Chemistry,* 6(2), 93-102.

[12] Bača M., Horváthová J., Mokrišová M. and Suhányiová A., (2015) On topological indices of fullerenes, *Applied Mathematics and Computation*, 251, 154–161.

[13] Bača M., Horváthová J., Mokrišová M., Semanicov-Fenovckov A. and Suhányiová A., (2015) On topological indices of carbon nanotube network, *Canadian Journal of Chemistry*, 93, 1–4.

[14] Dobrymin A.A., Gutman I., Klavžar S. and Zigert P., (2002) Wiener Index of Hexagonal Systems, *Acta Applicandae Mathematica*, 72(3), 247-294.

[15] Eliasi M., Iranmanesh A. and Gutman I., (2012) Multiplicative versions of first Zagreb index, *MATCH Communications in Mathematical and in Computer Chemistry*, 68(1), 217-230.

[16] Evarestov R.A., Zhukovskii Y.F., Bandura A.V. and Piskunov S., (2011) Symmetry and models of single-walled TiO2 nanotubes with rectangular morphology, *Central European Journal of Physics*, 9(2), 492–501.

[17] Gutman I. and Polansky O.E., (1986) Mathematical Concepts in Organic Chemistry, *Springer-Verlag*, Berlin, Germany.

[18] Gutman I., (2013) Degree-Based Topological Indices, *Croatica Chemica Acta*, 86(4), 351–361.

[19] Hayat S. and Imran M., (2014) Computation of topological indices of certain networks, *Applied Mathematics and Computation*, 240, 213–228.

[20] Hayat S., Imran M., (2015) On Degree Based Topological Indices of Certain Nanotubes, *Journal of Computational and Theoretical Nanoscience*, 12(8), 1599-1605

[21] Imran M., Hayat S. and Mailk M.Y.H., (2014) On topological indices of certain interconnection networks, *Applied Mathematics and Computation*, 244, 936–951.

[22] Gao W., Farahani M.R., Imran M., (2017) About the Randić connectivity, modify Randić connectivity and sum-connectivity indices of titania nanotubes Tio_2(m,n). *Acta Chim. Slov.* 64(1), 256–260.

[23] Farahani M.R., Pradeep Kumar R., Rajesh Kanna M.R., Wang S., (2016) The vertex Szeged index of Titania Carbon Nanotubes TiO_2(m,n). *International Journal of Pharmaceutical sciences and Research.* 7(9), 3734-3741.

[24] Farahani M.R., Jamil M.K., Pradeep Kumar R., Rajesh Kanna M. R., (2016) Computing Edge Co-Padmakar-Ivan Index of Titania TiO_2(m,n). *Journal of Environmental Science, Computer Science and Engineering & Technology*. 5(3), 326-334.

[25] Farahani M.R., Jamil M.K., Imran M., (2016) Vertex PIv topological index of Titania carbon Nanotubes, *Applied Mathematics and Nonlinear Sciences*, 1(1), 170-176.

[26] Huo Y., Liu J.-B., Imran M., Saeed M., Farahani M.R., Iqbal M.A., Malik M.A., (2016) On Some Degree-Based Topological Indices of Line Graphs of TiO_2[m,n] Nanotubes, *Journal of Computational and Theoretical Nanoscience*, 13(12), 9131–9135.

[27] H. Jiang, Jamil M.K., Siddiqui M.K., Farahani M.R., Shao Z., (2017) Edge-Vertex Szeged Index of Titania Nanotube TiO_2 (m,n),m,n>1. *International Journal of Advanced Biotechnology and Research.* 8(2), 1590-1597.

[28] Gao W., Liu J.B., Siddiqui M.K., Farahani M.R., (2016) Computing three topological indices for Titania Nanotubes TiO_2[m;n]. *AKCE International Journal of Graphs and Combinatorics,* 13(3), 255–260.

[29] Gao W., Farahani M.R., Jamil M.K., Siddiqui M.K., (2016) The Redefined First, Second and Third Zagreb Indices of Titania Nanotubes TiO_2[m,n]. *The Open Biotechnology Journal,* 10, 272-277.

[30] Gao W., Jamil M.K., Farahani M.R., Imran M., (2016) Certain topological indices of Titania TiO_2(m,n). *Journal of Computational and Theoretical Nanoscience,* 13(10), 7324–7328.

[31] Li Y., Yan L., Farahani M.R., Imran M.,, Jamil M.K., (2017) Computing the Theta Polynomial and the Theta Index of Titania Nanotubes TiO_2(m,n), *Journal of Computational and Theoretical Nanoscience,* 14(1), 715–717.

[32] Yan L., Li Y., Farahani M.R., Imran M., (2016) Sadhana and Pi polynomials and their indices of an infinite class of the Titania Nanotubes TiO_2(m,n). *Journal of Computational and Theoretical Nanoscience,* 13(11), 8772–8775.

[33] Yan L., Li Y., Farahani M.R., Jamil M.K., (2016) The Edge-Szeged index of the Titania Nanotubes TiO_2(m,n). *International Journal of Biology, Pharmacy and Allied Sciences.* 5(6), 1260-1269.

[34] Yan L., Li Y., S. Hayat, Afzal Siddiqui H.M., Imran M., Ahmad S., Farahani M.R., (2016) On degree-based and frustration related topological indices of single-walled titania nanotubes. *Journal of Computational and Theoretical Nanoscience,* 13(11), 9027–9032.

[35] Liu Y., Rezaei M., Husin M.N., Farahani M.R., Imran M., (2017) The Omega polynomial and the Cluj-Ilmenau index of an infinite class of the Titania Nanotubes Tio_2(m,n). *Journal of Computational and Theoretical Nanoscience,* 14(7), 3429–3432.

[36] Rezaei M., Farahani M.R., Jamil M.K., Ali K., Lee D.W., (2016) Vertex Version of Co-PI index of Titania Nanotubes TiO_2. *Advances and Applications in Mathematical*. 15(8), 255-262.

[37] Malik M.A. and Imran M., (2015) On multiple Zagreb index of TiO2 nanotubes, Acta Chimica Slovenica, 62, 973–976.