

Some polynomials and degree-based topological indices of molecular graph and line graph of Titanium dioxide nanotubes

Jaber Ramezani Tousi [†]

Masoud Ghods ^{*}

Department of Applied Mathematics

Semnan University

Semnan 35131-19111

Iran

Abstract

Graph polynomials based on distance and degree are helpful and necessary because they contain much information about topological indices.

In this article, the general inverse sum indeg index and the generalized inverse sum indeg polynomials are calculated for the molecular graph and the line graph of the Titanium dioxide nanotubes. Then, with their help, some polynomials and some degree-based topological indices of the molecular graph and the line graph of Titanium dioxide nanotubes are obtained.

Subject Classification: (2010) 05C90, 05C07, 92E20, 82D80, 92E10.

Keywords: Topological indices, Polynomial, Titanium dioxide nanotubes, Line graph, Molecular graph.

1. Introduction

Graph theory is used in chemistry for modeling. Study in nanoscale leads to drastic changes in material properties. Numerical calculations are of particular importance in nanoscale simulations.

Suppose $G = (V, E)$ is a simple and connected graph. We represent the set of edges with $E(G)$ and the number of edges with $|E(G)|$ and the set of vertices with $V(G)$, and the number of vertices with $|V(G)|$.

In graph G , we denote the degree of vertex u by d_u and if there is an edge between two vertices u and v , denoted it by $uv \in E(G)$.

[†] E-mail: jaber.ramezani@semnan.ac.ir

^{*} E-mail: mghods@semnan.ac.ir (Corresponding Author)

In a molecular graph, the topological index is expressed as an actual number, and this number is attributed to the graphs, uniform with that molecule. The topological index also indicates some of the properties of the molecule.

Definition 1.1: The general inverse sum indeg index of a graph G , denoted by $ISI_{(\alpha,\beta)}(G)$, and defined as [4]:

$$ISI_{(\alpha,\beta)}(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha (d_u + d_v)^\beta$$

Some degree-based indices of graph G can be obtained from the generalized $ISI_{(\alpha,\beta)}(G)$ index by assigning specific values to the parameters α and β (see Table 1). For details, see [6, 8, 10, 11], and the references cited therein.

Table 1
Some topological index definition and Corresponding $ISI_{(\alpha,\beta)}(G)$.

Topological index	Topological index definition	Corresponding $ISI_{(\alpha,\beta)}(G)$
First Zagreb index	$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$	$ISI_{(0,1)}(G)$
Second Zagreb index	$M_2(G) = \sum_{uv \in E(G)} (d_u d_v)$	$ISI_{(1,0)}(G)$
Randic index	$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$	$ISI_{(-\frac{1}{2},0)}(G)$
Sum connectivity index	$SCI(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$	$ISI_{(0,-\frac{1}{2})}(G)$
Harmonic index	$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$	$2ISI_{(0,-1)}(G)$
Hyper Zagreb index	$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2$	$ISI_{(0,2)}(G)$
Redefined third Zagreb index	$ReZG_3(G) = \sum_{uv \in E(G)} (d_u d_v)(d_u + d_v)$	$ISI_{(1,1)}(G)$
Geometric Arithmetic index	$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$	$2ISI_{(\frac{1}{2},-1)}(G)$
Inverse sum indeg index	$ISI(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}$	$ISI_{(1,-1)}(G)$
General sum connectivity index	$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha$	$ISI_{(0,\alpha)}(G)$
Generalized Randić' index	$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$	$ISI_{(\alpha,0)}(G)$

Different topological indices can be obtained with the help of polynomials by point quantification directly or by taking integrals or derivatives.

Definition 1.2: In a non-empty graph G , if each edge is considered as a vertex and the two vertices are connected, if the corresponding edges of the two vertices are adjacent to G , the resulting graph is denoted by $L(G)$ and is called the line graph of G [2].

Definition 1.3: The generalized inverse sum indeg polynomial of a graph G , denoted by $ISI_{(\alpha, \beta)}(G, x)$, and defined as [3]:

$$ISI_{(\alpha, \beta)}(G, x) = \sum_{uv \in E(G)} x^{(d_u d_v)^\alpha (d_u + d_v)^\beta},$$

Where α and β are some real numbers (see Table 2).

Table 2 shows the relationships between generalized inverse sum indeg polynomial and other polynomials associated with topological indices [12].

Table 2
Polynomials associated with Topological indices and Corresponding
 $ISI_{(\alpha, \beta)}(G, x)$.

Polynomials associated with Topological indices	Polynomial definition	Corresponding $ISI_{(\alpha, \beta)}(G, x)$
First Zagreb polynomial	$M_1(G, x) = \sum_{uv \in E(G)} x^{(d_u + d_v)}$	$ISI_{(0,1)}(G, x)$
Second Zagreb polynomial	$M_2(G, x) = \sum_{uv \in E(G)} x^{(d_u d_v)}$	$ISI_{(1,0)}(G, x)$
Hyper Zagreb polynomial	$HM(G, x) = \sum_{uv \in E(G)} x^{(d_u + d_v)^2}$	$ISI_{(0,2)}(G, x)$
Redefined third Zagreb polynomial	$ReZG_3(G, x) = \sum_{uv \in E(G)} x^{(d_u d_v)(d_u + d_v)}$	$ISI_{(1,1)}(G, x)$
General sum connectivity polynomial	$\chi_\alpha(G, x) = \sum_{uv \in E(G)} x^{(d_u + d_v)^\alpha}$	$ISI_{(0, \alpha)}(G, x)$
Generalized Randić' polynomial	$R_\alpha(G, x) = \sum_{uv \in E(G)} x^{(d_u d_v)^\alpha}$	$ISI_{(\alpha, 0)}(G, x)$

2. The structure of the molecular graph and the line graph of the Titanium dioxide nanotube

Titanium dioxide nanotubes, abbreviated as $TiO_2[m, n]$, are one of the most essential and practical compounds in materials science that have many applications in the production of catalytic materials, gas sensors, biomedical devices, solar cells, etc.

One of the characteristics of Titanium dioxide nanotube sheets is the considerable stability of its atomic multilayer sheets [5]. Malik et. al. calculated the Zagreb indices in Titanium dioxide nanotubes [7]. Recently, A. Ahmad et. al. computed the degree-based topological indices of the line graph of benzene ring [1]. Also, Raheem et. al. used M-Polynomials to calculate topological indices in Titanium dioxide [9].

The molecular graph of $TiO_2[m, n]$ nanotubes is shown in Figure 1, where m represents the number of octagons in a row and n represents the number of octagons in a column of Titanium dioxide nanotubes.

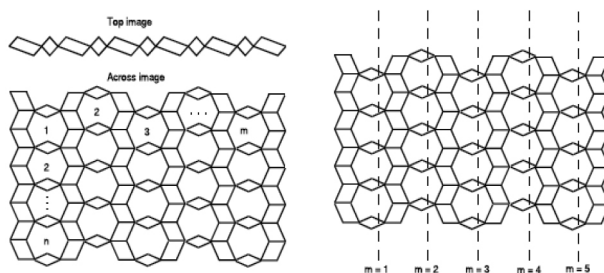


Figure 1

The molecular graph of $TiO_2[m, n]$.

In this article, the molecular graph of Titanium dioxide nanotubes is denoted by G , its line graph by G' . There are four types of edges in the molecular graph of Titanium dioxide nanotubes:

$$E_1 = \{(d_u, d_v) | uv \in E(G), d_u = 2, d_v = 4\}, E_2 = \{(d_u, d_v) | uv \in E(G), d_u = 2, d_v = 5\},$$

$$E_3 = \{(d_u, d_v) | uv \in E(G), d_u = 3, d_v = 4\}, E_4 = \{(d_u, d_v) | uv \in E(G), d_u = 3, d_v = 5\}.$$

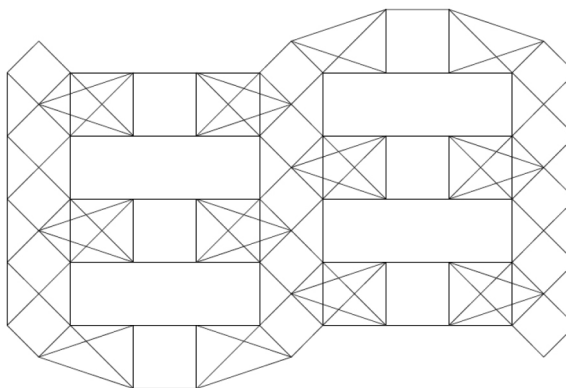
According to Figure 1, we have the following Table 3 for the molecular graph of Titanium dioxide nanotubes:

Table 3

The number of edges in the molecular graph of Titanium dioxide nanotubes.

Edge type	Number of edges	$d_u d_v$	$d_u + d_v$
E_1	$6m+2$	8	6
E_1	$4mn+2m+2$	10	7
E_1	$2m+2$	12	7
E_1	$6mn+6n-2m-2$	15	8

The status of the rows and columns in the molecular graph of the Titanium dioxide nanotube is shown in Figure 2.


Figure 2

The line graph of the Titanium dioxide nanotube.

There are ten types of edges in line graph of Titanium dioxide nanotubes:

$$\begin{aligned}
 E'_1 &= \{(d_u, d_v) \mid uv \in E(G'), d_u = 2, d_v = 3\}, & E'_2 &= \{(d_u, d_v) \mid uv \in E(G'), d_u = 2, d_v = 5\}, \\
 E'_3 &= \{(d_u, d_v) \mid uv \in E(G'), d_u = 3, d_v = 4\}, & E'_4 &= \{(d_u, d_v) \mid uv \in E(G'), d_u = 3, d_v = 6\}, \\
 E'_5 &= \{(d_u, d_v) \mid uv \in E(G'), d_u = 4, d_v = 4\}, & E'_6 &= \{(d_u, d_v) \mid uv \in E(G'), d_u = 4, d_v = 5\}, \\
 E'_7 &= \{(d_u, d_v) \mid uv \in E(G'), d_u = 4, d_v = 6\}, & E'_8 &= \{(d_u, d_v) \mid uv \in E(G'), d_u = 5, d_v = 5\}, \\
 E'_9 &= \{(d_u, d_v) \mid uv \in E(G'), d_u = 5, d_v = 6\}, & E'_{10} &= \{(d_u, d_v) \mid uv \in E(G'), d_u = 6, d_v = 6\}.
 \end{aligned}$$

According to Figure 2, we have the following Table 4 for the line graph of Titanium dioxide nanotubes.

Table 4
The number of edges in the line graph of Titanium dioxide nanotubes.

Edge type	Number of edges	$d_u d_v$	$d_u + d_v$
E'_1	2	6	5
E'_2	2	10	7
E'_3	8	12	7
E'_4	2	18	9
E'_5	$8m+8n-6$	16	8
E'_6	$8m$	20	9
E'_7	$8n-4$	24	10
E'_8	$4mn+4m$	25	10
E'_9	$24mn-10m$	30	11
E'_{10}	$11mn-4m-5n$	36	12

3. Main Results

Given that in the molecular graph of Titanium dioxide nanotubes, there are always $\delta(G) = 2$ and $\Delta(G) = 5$, so for each arbitrary vertex u , we have:

$$2 \leq d_u \leq 5.$$

Theorem 3.1: Let G be the molecular graph of Titanium dioxide nanotubes. Then

$$\begin{aligned} ISI_{(\alpha, \beta)}(G) &= (6m+2)(8)^\alpha 6^\beta + (4mn+2m+2)(10)^\alpha 7^\beta \\ &\quad + (2m+2)(12)^\alpha 7^\beta + (6mn+6n-2m-2)(15)^\alpha 8^\beta. \end{aligned}$$

Proof:

$$\begin{aligned} ISI_{(\alpha, \beta)}(G) &= \sum_{uv \in E(G)} [d_u d_v]^\alpha [d_u + d_v]^\beta \\ &= \sum_{uv \in E_1} [d_u d_v]^\alpha [d_u + d_v]^\beta + \sum_{uv \in E_2} [d_u d_v]^\alpha [d_u + d_v]^\beta \\ &\quad + \sum_{uv \in E_3} [d_u d_v]^\alpha [d_u + d_v]^\beta + \sum_{uv \in E_4} [d_u d_v]^\alpha [d_u + d_v]^\beta \\ &= (6m+2)(8)^\alpha 6^\beta + (4mn+2m+2)(10)^\alpha 7^\beta + (2m+2)(12)^\alpha 7^\beta \\ &\quad + (6mn+6n-2m-2)(15)^\alpha 8^\beta. \end{aligned}$$

Theorem 3.2: Suppose that G is the molecular graph of Titanium dioxide nanotubes. Then

- i. $M_1(G) = 76mn + 48m + 48n + 24$,
- ii. $M_2(G) = 130mn + 62m + 9n + 30$,
- iii. $R(G) = 2.8141mn + 2.8147m + 1.5492n + 1.4005$,
- iv. $SCI(G) = 3.6332mn + 3.2542m + 2.1213n + 0.6808$,
- v. $H(G) = 1.3304mn + 3.0804m + 0.1875n + 1.747$,
- vi. $HM(G) = 0.1754mn + 0.2170m + 0.09375n + 0.1059$,
- vii. $ReZG_3(G) = 352mn + 356m + 72n + 164$,
- viii. $GA(G) = 9.4236mn + 7.3344m + 5.8094n + 3.5632$,
- ix. $ISI(G) = 16.9643mn + 9.9643m + 11.25n + 4.6309$,
- x. $\chi_\alpha(G) = (6m + 2)6^\alpha + (4mn + 2m + 2)7^\alpha + (2m + 2)7^\alpha$
 $+ (6mn + 6n - 2m - 2)8^\alpha$,
- xi. $R_\alpha(G) = (6m + 2)(8)^\alpha + (4mn + 2m + 2)(10)^\alpha + (2m + 2)(12)^\alpha$
 $+ (6mn + 6n - 2m - 2)(15)^\alpha$.

Proof: By using the relations in Table 1 and placing them in Theorem 3.1, the proof is complete.

Theorem 3.3: Let G be the molecular graph of Titanium dioxide nanotubes. Then the general inverse sum indeg polynomial of G is given by

$$ISI_{(\alpha, \beta)}(G, x) = (6m + 2)x^{(8)^\alpha 6^\beta} + (4mn + 2m + 2)x^{(10)^\alpha 7^\beta} \\ + (2m + 2)x^{(12)^\alpha 7^\beta} + (6mn + 6n - 2m - 2)x^{(15)^\alpha 8^\beta}.$$

Proof:

$$ISI_{(\alpha, \beta)}(G, x) = \sum_{uv \in E(G)} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} \\ = \sum_{uv \in E_1} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} + \sum_{uv \in E_2} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} + \sum_{uv \in E_3} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} \\ + \sum_{uv \in E_4} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} \\ = (6m + 2)x^{(8)^\alpha 6^\beta} + (4mn + 2m + 2)x^{(10)^\alpha 7^\beta} + (2m + 2)x^{(12)^\alpha 7^\beta} \\ + (6mn + 6n - 2m - 2)x^{(15)^\alpha 8^\beta}.$$

Theorem 3.4: Let G be molecular graph of Titanium dioxide nanotubes. Then

- i. $M_1(G, x) = (6m+2)x^6 + (4mn+2m+2)x^7 + (2m+2)x^8 + (6mn+6n-2m-2)x^8,$
- ii. $M_2(G, x) = (6m+2)x^8 + (4mn+2m+2)x^{10} + (2m+2)x^{12} + (6mn+6n-2m-2)x^{15},$
- iii. $HM(G, x) = (6m+2)x^{36} + (4mn+2m+2)x^{49} + (2m+2)x^{49} + (6mn+6n-2m-2)x^{64},$
- iv. $ReZG_3(G, x) = (6m+2)x^{48} + (4mn+2m+2)x^{70} + (2m+2)x^{84} + (6mn+6n-2m-2)x^{120},$
- v. $\chi_\alpha(G, x) = (6m+2)x^{6^\alpha} + (4mn+2m+2)x^{7^\alpha} + (2m+2)x^{7^\alpha} + (6mn+6n-2m-2)x^{8^\alpha},$
- vi. $R_\alpha(G, x) = (6m+2)x^{8^\alpha} + (4mn+2m+2)x^{10^\alpha} + (2m+2)x^{12^\alpha} + (6mn+6n-2m-2)x^{15^\alpha}.$

Proof: By using the relations in Table 2 and placing them in Theorem 3.3, the proof is complete.

Theorem 3.5: Let G' be line graph of Titanium dioxide nanotubes. Then

$$\begin{aligned}
 ISI_{(\alpha, \beta)}(G') &= (2)(6)^\alpha 5^\beta + (2)(10)^\alpha 7^\beta + (8)(12)^\alpha 7^\beta + (2)(18)^\alpha 9^\beta \\
 &\quad + (8m+8n-6)(16)^\alpha 8^\beta + (8m)(20)^\alpha 9^\beta + (8n-4)(24)^\alpha 10^\beta \\
 &\quad + (4mn+4m)(25)^\alpha 10^\beta + (24mn-10m)(30)^\alpha 11^\beta \\
 &\quad + (11mn-4m-5n)(36)^\alpha 12^\beta.
 \end{aligned}$$

Proof:

$$\begin{aligned}
 ISI_{(\alpha, \beta)}(G') &= \sum_{uv \in E(G')} [d_u d_v]^\alpha [d_u + d_v]^\beta \\
 &= \sum_{uv \in E'_1} [d_u d_v]^\alpha [d_u + d_v]^\beta + \sum_{uv \in E'_2} [d_u d_v]^\alpha [d_u + d_v]^\beta + \sum_{uv \in E'_3} [d_u d_v]^\alpha [d_u + d_v]^\beta \\
 &\quad + \sum_{uv \in E'_4} [d_u d_v]^\alpha [d_u + d_v]^\beta + \sum_{uv \in E'_5} [d_u d_v]^\alpha [d_u + d_v]^\beta + \sum_{uv \in E'_6} [d_u d_v]^\alpha [d_u + d_v]^\beta \\
 &\quad + \sum_{uv \in E'_7} [d_u d_v]^\alpha [d_u + d_v]^\beta + \sum_{uv \in E'_8} [d_u d_v]^\alpha [d_u + d_v]^\beta + \sum_{uv \in E'_9} [d_u d_v]^\alpha [d_u + d_v]^\beta \\
 &\quad + \sum_{uv \in E'_{10}} [d_u d_v]^\alpha [d_u + d_v]^\beta
 \end{aligned}$$

$$\begin{aligned}
 &= (2)(6)^\alpha 5^\beta + (2)(10)^\alpha 7^\beta + (8)(12)^\alpha 7^\beta + (2)(18)^\alpha 9^\beta + (8m + 8n - 6)(16)^\alpha 8^\beta \\
 &+ (8m)(20)^\alpha 9^\beta + (8n - 4)(24)^\alpha 10^\beta + (4mn + 4m)(25)^\alpha 10^\beta \\
 &+ (24mn - 10m)(30)^\alpha 11^\beta + (11mn - 4m - 5n)(36)^\alpha 12^\beta.
 \end{aligned}$$

Theorem 3.6: Suppose that G' is the line graph of Titanium dioxide nanotubes. Then

- i. $M_1(G') = 436mn + 18m + 84n + 10,$
- ii. $M_2(G') = 1216mn - 56m + 140n - 28,$
- iii. $R(G') = 7.999mn + 1.0964m + 2.7996n + 1.9133,$
- iv. $SCI(G') = 11.6766mn + 2.5902m + 3.9149n + 1.9545,$
- v. $H(G') = 6.997mn + 1.293m - 2.7666n + 1.8016,$
- vi. $HM(G') = 0.1246mn + 0.1533m + 0.1703n + 0.1750,$
- vii. $ReZG_3(G') = 13672mn - 1564m + 784n - 532,$
- viii. $GA(G') = 35.7006mn + 5.9918m + 10.8384n + 4.3738,$
- ix. $ISI(G') = 108.4545mn + 4.5050m + 20.2n + 1.3714,$
- x. $\chi_\alpha(G') = (2)5^\alpha + (10)7^\alpha + (8m + 8n - 6)8^\alpha + (8m + 2)9^\alpha + (4mn + 4m + 8n - 4)10^\alpha + (24mn - 10m)11^\alpha + (11mn - 4m - 5n)12^\alpha,$
- xi. $R_\alpha(G') = (2)(6)^\alpha + (2)(10)^\alpha + (8)(12)^\alpha + (2)(18)^\alpha + (8m + 8n - 6)(16)^\alpha + (8m)(20)^\alpha + (8n - 4)(24)^\alpha + (4mn + 4m)(25)^\alpha + (24mn - 10m)(30)^\alpha + (11mn - 4m - 5n)(36)^\alpha.$

Proof: By using the relations in Table 1 and placing them in Theorem 3.5, the proof is complete.

Theorem 3.7: Let G' be the line graph of Titanium dioxide nanotubes. Then the general inverse sum indeg polynomial of G' is given by

$$\begin{aligned}
 ISI_{(\alpha, \beta)}(G', x) &= (2)x^{(6)^\alpha 5^\beta} + (2)x^{(10)^\alpha 7^\beta} + (8)x^{(12)^\alpha 7^\beta} + (2)x^{(18)^\alpha 9^\beta} \\
 &+ (8m + 8n - 6)x^{(16)^\alpha 8^\beta} + (8m)x^{(20)^\alpha 9^\beta} + (8n - 4)x^{(24)^\alpha 10^\beta} \\
 &+ (4mn + 4m)x^{(25)^\alpha 10^\beta} + (24mn - 10m)x^{(30)^\alpha 11^\beta} \\
 &+ (11mn - 4m - 5n)x^{(36)^\alpha 12^\beta}.
 \end{aligned}$$

Proof:

$$\begin{aligned}
ISI_{(\alpha, \beta)}(G', x) &= \sum_{uv \in E(G')} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} \\
&= \sum_{uv \in E'_1} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} + \sum_{uv \in E'_2} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} + \sum_{uv \in E'_3} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} + \sum_{uv \in E'_4} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} \\
&+ \sum_{uv \in E'_5} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} + \sum_{uv \in E'_6} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} + \sum_{uv \in E'_7} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} + \sum_{uv \in E'_8} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} \\
&+ \sum_{uv \in E'_9} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} + \sum_{uv \in E'_{10}} x^{[d_u d_v]^\alpha [d_u + d_v]^\beta} \\
&= (2)x^{(6)^\alpha 5^\beta} + (2)x^{(10)^\alpha 7^\beta} + (8)x^{(12)^\alpha 7^\beta} + (2)x^{(18)^\alpha 9^\beta} + (8m+8n-6)x^{(16)^\alpha 8^\beta} \\
&+ (8m)x^{(20)^\alpha 9^\beta} + (8n-4)x^{(24)^\alpha 10^\beta} + (4mn+4m)x^{(25)^\alpha 10^\beta} + (24mn-10m)x^{(30)^\alpha 11^\beta} \\
&+ (11mn-4m-5n)x^{(36)^\alpha 12^\beta}.
\end{aligned}$$

Theorem 3.8: Let G' be the line graph of Titanium dioxide nanotubes. Then

- i. $M_1(G', x) = 2x^5 + 10x^7 + (8m+8n-6)x^8 + (8m+2)x^9 + (4mn+4m+8n-4)x^{10} + (24mn-10m)x^{11} + (11mn-4m-5n)x^{12},$
- ii. $M_2(G', x) = 2x^6 + 2x^{10} + 8x^{12} + 2x^{18} + (8m+8n-6)x^{16} + (8m)x^{20} + (8n-4)x^{24} + (4mn+4m)x^{25} + (24mn-10m)x^{30} + (11mn-4m-5n)x^{36},$
- iii. $HM(G', x) = 2x^{25} + 10x^{49} + (8m+8n-6)x^{64} + (8m+2)x^{81} + (4mn+4m+8n-4)x^{100} + (24mn-10m)x^{121} + (11mn-4m-5n)x^{144},$
- iv. $Re ZG_3(G', x) = 2x^{30} + 2x^{70} + 8x^{84} + 2x^{162} + (8m+8n-6)x^{128} + (8m)x^{180} + (8n-4)x^{240} + (4mn+4m)x^{250} + (24mn-10m)x^{330} + (11mn-4m-5n)x^{432},$
- v. $\chi_\alpha(G', x) = 2x^{5^\alpha} + 10x^{7^\alpha} + (8m+8n-6)x^{8^\alpha} + (8m+2)x^{9^\alpha} + (4mn+4m+8n-4)x^{10^\alpha} + (24mn-10m)x^{11^\alpha} + (11mn-4m-5n)x^{12^\alpha},$
- vi. $R_\alpha(G', x) = 2x^{(6)^\alpha} + 2x^{(10)^\alpha} + 8x^{(12)^\alpha} + 2x^{(18)^\alpha} + (8m+8n-6)x^{(16)^\alpha} + (8m)x^{(20)^\alpha} + (8n-4)x^{(24)^\alpha} + (4mn+4m)x^{(25)^\alpha} + (24mn-10m)x^{(30)^\alpha} + (11mn-4m-5n)x^{(36)^\alpha}.$

Proof: By using the relations in Table 2 and placing them in Theorem 3.7, the proof is complete.

4. Conclusion

In this article, with the help of the general inverse sum indeg index and the generalized inverse sum indeg polynomial, some important polynomials were obtained in the molecular graph and line graph of Titanium dioxide nanotubes, and some degree-based topological indices were also calculated. According to the structure of Titanium Dioxide, all indices were obtained in terms of m and n . This method can also be used for other nanotubes.

5. Acknowledgements

The authors are very grateful to the editor and the anonymous referee(s) for their comments and suggestions which led to the present improved version of the manuscript.

References

- [1] Ahmad, A., Elahi, K., Hasni, R. & Nadeem, M. F., "Computing the degree based topological indices of line graph of benzene ring embedded in P-type-surface in 2D network", *Journal of Information and Optimization Sciences*, 40:7, (2019), 1511-1528, DOI: 10.1080/02522667.2018.1552411.
- [2] Alameri, A., "Second Hyper Zagreb Index of Titanium dioxide Nanotubes and Their Applications", *IEEE Access*, Vol. 9, (2021).
- [3] Ali, P., Kirmani, S. A. K., Al Rugaie, O., Azam, F., "Degree-based topological indices and polynomials of hyaluronic acid-curcumin conjugates", *Saudi Pharmaceutical Journal*, (2020).
- [4] Bharali, A., Pegu, A., & Buragohain, J., Deka, B., "Generalized ISI index of certain families of nanostar dendrimers", *Journal of Interdisciplinary Mathematics*, 24, (2021).
- [5] Evarestov, R. A., Zhukovskii, Y.F., Bandura, A.V., Piskunov, S., "Symmetry and models of single walled TiO₂ [m, n] nanotubes with rectangular morphology", *Cent. Eur. J. Phys*, 9 (2), (2011), 492–501.
- [6] Kulli, V. R., Pal, M., Samanta, S., Pal A., "Handbook of Research of Advanced Applications of Graph Theory in Modern Society", Global, Hershey, (2020).
- [7] Malik, M.A., Imran, M., "On multiple Zagreb index of TiO₂ nanotubes, "Acta Chim. Slov", 62 (4), (2015) 973–976.

- [8] Milovanovic, I., Milovanovic, E., Matejic, M., "On some mathematical properties of Sombor indices", *Bull. Int. Math. Virtual Inst*, 11, (2021), 341–353.
- [9] Raheem, A., Javaid, M., Teh, W. C., Wang, S., Liu, J., "M-polynomial method for topological indices of 2D-lattice of three-layered single-walled Titanium dioxide nanotubes", *Journal of Information and Optimization Sciences*, 41:3, (2020) 743-753.
- [10] Redzepovic, I., "Chemical applicability of Sombor indices", *J. Serb. Chem. Soc*, 86, (2021), 445–457.
- [11] Todeschini, R., Consonni, V., "Molecular Descriptors for Chemoinformatics", Wiley, VCH, Weinheim, (2009).
- [12] Vetrík, T., "Polynomials of degree-based indices for hexagonal nanotubes", *UPB Sci. Bull. Ser. B Chem. Mater. Sci*, 81, (2019), 109–120.

Received February, 2022

Revised July, 2022