POLYNOMIALS OF DEGREE-BASED INDICES FOR HEXAGONAL NANOTUBES

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In theoretical chemistry, topological indices are used for modelling properties of chemical compounds and biological activities in chemistry, biochemistry and nanotechnology. Topological indices of nanotubes are numerical descriptors which are derived from graphs of chemical compounds. These indices are extensively used for establishing relationships between the structure of nanotubes and their physico-chemical properties.

One or a few chosen polynomials of topological indices for nanotubes have been studied in several papers. We give general formulas and use them to obtain any polynomial of degree-based indices for hexagonal nanotubes. We also show that the derivatives of these polynomials can be used to obtain various topological indices such as the general Randić index for hexagonal nanotubes.

Keywords: degree-based index, polynomial, nanotube.

1. Introduction

Hexagonal nanotubes are allotropes of carbon with a cylindrical nanostructure. These cylindrical carbon molecules have interesting properties, that are valuable for nanotechnology, optics, electronics and other fields of materials science and technology. Hexagonal nanotubes have exceptional thermal conductivity, electrical and mechanical properties. They have applications as additives to numerous structural materials. Carbon nanotubes are the strongest and stiffest materials yet discovered with respect to elastic modulus and tensile strength. They are either metallic or semiconducting along the tubular axis. Hexagonal nanotubes have useful absorption and they belong to the most important compounds in materials science.

In theoretical chemistry, topological indices are used for modelling properties of chemical compounds and biological activities in chemistry, biochemistry and nanotechnology. Topological indices of nanotubes are numerical descriptors which are derived from graphs of chemical compounds. It was described for example in [7] that these indices are extensively used for establishing relationships between the structure of nanotubes and their physico-chemical properties. Topological indices for hexagonal nanotubes have been studied for

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about 15 years. The first works include [4] and [8]. Since then, hundreds of papers have been published on topological indices for nanotubes.

Topological indices are often studied with the help of their polynomials. The first Zagreb polynomial and the second Zagreb polynomial for hexagonal nanotubes were given in [5]. The first Zagreb polynomial, the second Zagreb polynomial and the forgotten polynomial of generalized prisms and toroidal polyhex networks were computed in [1] and Zagreb polynomials of nanostars were computed in [9, 12]. The harmonic polynomial of polycyclic aromatic hydrocarbons was studied in [6]. Polynomials of various networks were studied also in [10, 11] and hexagonal nanotubes were investigated for example in [2, 3, 13]. We give two formulas and use them to obtain any polynomial of degree-based indices for hexagonal nanotubes.

2. General degree-based indices and their polynomials

Let Γ be a graph with the vertex set $V(\Gamma)$ and the edge set $E(\Gamma)$. Vertices correspond to the atoms of a compound and edges correspond to chemical bonds. The degree d_u of a vertex $u \in V(\Gamma)$ is the number of neighbours of u.

The most general indices based on degrees are the general Randić index of a graph Γ,

$$R_\alpha(\Gamma) = \sum_{vu \in E(\Gamma)} (d_v d_u)^\alpha,$$

the general sum-connectivity index

$$X_\alpha(\Gamma) = \sum_{vu \in E(\Gamma)} (d_v + d_u)^\alpha$$

and the generalized Zagreb index

$$GZ_{\alpha,\beta}(\Gamma) = \sum_{vu \in E(\Gamma)} d_v^\alpha d_u^\beta + d_u^\alpha d_v^\beta.$$

Note that the third redefined Zagreb index is defined as

$$ReZ(\Gamma) = \sum_{vu \in E(\Gamma)} d_v d_u (d_v + d_u)$$

and the harmonic index is defined as

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

Let us introduce a general invariant

$$P(\Gamma, x) = \sum_{vu \in E(\Gamma)} x^{g(d_v, d_u)},$$

where $g(d_v, d_u)$ is a function of d_v and d_u, and $g(d_v, d_u) = g(d_u, d_v)$. This invariant includes polynomials of topological indices defined above.

- If $g(d_v, d_u) = (d_v d_u)^\alpha$ where α is a positive integer, then $P(\Gamma, x)$ is the general Randić polynomial of Γ. Moreover, $P(\Gamma, x)$ is the second Zagreb polynomial if $\alpha = 1$.
- If $g(d_v, d_u) = (d_v + d_u)^\alpha$ where α is a positive integer, then $P(\Gamma, x)$ is the general sum-connectivity polynomial of Γ. Furthermore, $P(\Gamma, x)$ is the first Zagreb polynomial for $\alpha = 1$ and the hyper-Zagreb polynomial for $\alpha = 2$.
- If $g(d_v, d_u) = d_v^\alpha d_u^\beta + d_u^\alpha d_v^\beta$ where α is a positive integer and β is a non-negative integer, then $P(\Gamma, x)$ is the generalized Zagreb polynomial of Γ. Moreover, $P(\Gamma, x)$ is the forgotten polynomial if $\alpha = 2$ and $\beta = 0$.
- If $g(d_v, d_u) = d_v d_u (d_v + d_u)$, then $P(\Gamma, x)$ is the third redefined Zagreb polynomial of Γ.
- If $g(d_v, d_u) = d_v + d_u - 1$, then $P(\Gamma, x)$ is one half of the harmonic polynomial $H(\Gamma, x)$ of Γ. Note that the harmonic polynomial is defined differently from the other polynomials.

So the general Randić polynomial of any graph Γ is defined as

$$R_\alpha(\Gamma, x) = \sum_{vu \in E(\Gamma)} x^{(d_v d_u)^\alpha},$$

the general sum-connectivity polynomial is

$$X_\alpha(\Gamma, x) = \sum_{vu \in E(\Gamma)} x^{(d_v + d_u)^\alpha},$$

the generalized Zagreb polynomial of any graph Γ,

$$GZ_{\alpha,\beta}(\Gamma, x) = \sum_{vu \in E(\Gamma)} x^{d_v^\alpha d_u^\beta + d_u^\alpha d_v^\beta},$$

the third redefined Zagreb polynomial is defined as

$$ReZ(\Gamma, x) = \sum_{vu \in E(\Gamma)} x^{d_v d_u (d_v + d_u)}$$

and the harmonic polynomial is

$$H(\Gamma, x) = 2 \sum_{vu \in E(\Gamma)} x^{d_v + d_u - 1}.$$

3. **Armchair polyhex nanotubes**

The armchair polyhex nanotube $TUAC_6[p; q]$ for $q = 7$ and $p = 10$ is given in Figure 1. The number of hexagons in every column of the corresponding two-dimensional lattice is q and the number of hexagons in every row is p. Clearly, q can be any positive integer and p is even; see Figure 1.

We can obtain any polynomial of indices based on degrees for armchair polyhex nanotubes using the following theorem.

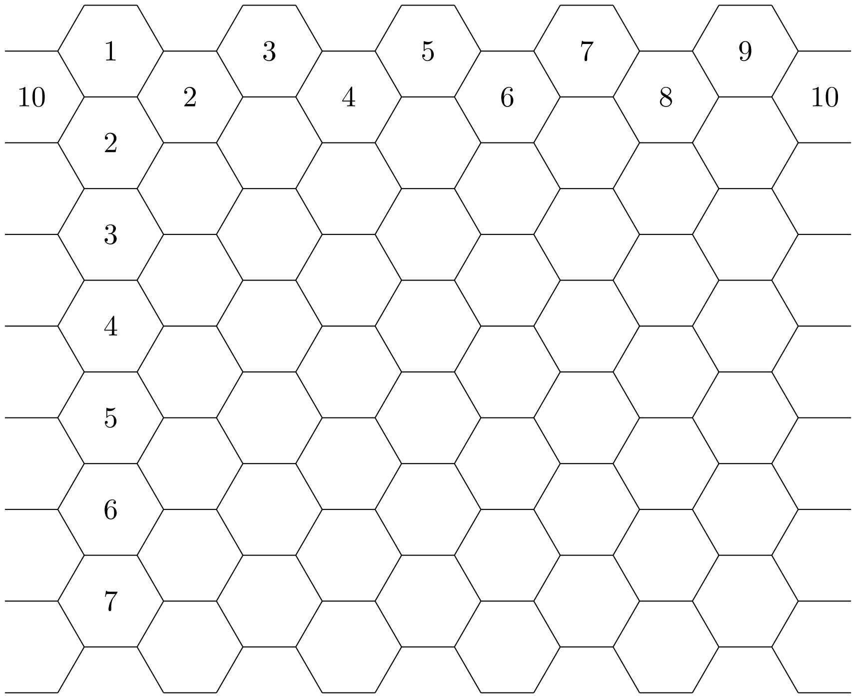

Fig. 1. Armchair polyhex nanotube $TUAC_6[p;q]$ for $q = 7$ and $p = 10$.

Theorem 3.1. *For the armchair polyhex nanotube* $\Gamma = TUAC_6[p;q]$, *we have*

$$P(\Gamma, x) = \sum_{vu \in E(\Gamma)} x^{g(d_v, d_u)} = (3q-1)p \cdot x^{g(3,3)} + 2p \cdot x^{g(3,2)} + p \cdot x^{g(2,2)}.$$

Proof. The armchair polyhex nanotube $TUAC_6[p;q]$ contains $(q+1)2p$ vertices and $(3q+2)p$ edges. Each vertex has degree either two or three (see Figure 1). Vertices of Γ can be divided into the sets. The set of vertices of degree 2,

$$V_2 = \{u \in V(\Gamma) \mid d_u = 2\},$$

and the set of vertices of degree 3,

$$V_3 = \{u \in V(\Gamma) \mid d_u = 3\}.$$

Since $|V_2| = 2p$, we obtain $|V_3| = |V(\Gamma)| - |V_2| = 2qp$. Let

$$\begin{aligned} E_{2,2} &= \{vu \in E(\Gamma) \mid d_v = d_u = 2\}, \\ E_{3,2} &= \{vu \in E(\Gamma) \mid d_v = 3,\ d_u = 2\}, \\ E_{3,3} &= \{vu \in E(\Gamma) \mid d_v = d_u = 3\}. \end{aligned}$$

Note that $E(\Gamma) = E_{2,2} \cup E_{3,2} \cup E_{3,3}$. The number of edges incident to two vertices of degree 2 is p, so $|E_{2,2}| = p$. Each vertex having degree two is adjacent to one vertex having degree three, thus we get $|E_{3,2}| = 2p$ and $|E_{3,3}| =$

$|E(\Gamma)| - |E_{2,2}| - |E_{3,2}| = (3q-1)p$. Hence,

$$\begin{aligned} P(\Gamma, x) &= \sum_{vu \in E(\Gamma)} x^{g(d_v,d_u)} = \sum_{vu \in E_{3,3}} x^{g(3,3)} + \sum_{vu \in E_{3,2}} x^{g(3,2)} + \sum_{vu \in E_{2,2}} x^{g(2,2)} \\ &= (3q-1)p \cdot x^{g(3,3)} + 2p \cdot x^{g(3,2)} + p \cdot x^{g(2,2)}. \end{aligned}$$

□

Polynomials of indices based on degrees for armchair polyhex nanotube are given in Corollary 3.1.

Corollary 3.1. *For the armchair polyhex nanotube* $\Gamma = TUAC_6[p;q]$*, we have the general Randić polynomial of* Γ*,*

$$R_\alpha(\Gamma, x) = (3q-1)px^{9^\alpha} + 2px^{6^\alpha} + px^{4^\alpha},$$

the second Zagreb polynomial

$$R_1(\Gamma, x) = (3q-1)px^9 + 2px^6 + px^4,$$

the general sum-connectivity polynomial of Γ*,*

$$X_\alpha(\Gamma, x) = (3q-1)px^{6^\alpha} + 2px^{5^\alpha} + px^{4^\alpha},$$

the first Zagreb polynomial

$$X_1(\Gamma, x) = (3q-1)px^6 + 2px^5 + px^4,$$

the hyper-Zagreb polynomial

$$X_2(\Gamma, x) = (3q-1)px^{36} + 2px^{25} + px^{16},$$

the generalized Zagreb polynomial of Γ*,*

$$GZ_{\alpha,\beta}(\Gamma, x) = (3q-1)px^{2\cdot 3^{\alpha+\beta}} + 2px^{2^\alpha 3^\beta + 3^\alpha 2^\beta} + px^{2^{\alpha+\beta+1}},$$

the forgotten polynomial

$$GZ_{2,0}(\Gamma, x) = (3q-1)px^{18} + 2px^{13} + px^8,$$

the third redefined Zagreb polynomial

$$ReZ(\Gamma, x) = (3q-1)px^{54} + 2px^{30} + px^{16}$$

and the harmonic polynomial

$$H(\Gamma, x) = (3q-1)2px^5 + 4px^4 + 2px^3.$$

Proof. For $R_\alpha(\Gamma, x)$ which is the general Randić polynomial of Γ we have $g(d_v, d_u) = (d_v d_u)^\alpha$, therefore $g(3,3) = 9^\alpha$, $g(3,2) = 6^\alpha$ and $g(2,2) = 4^\alpha$. So from Theorem 3.1,

$$R_\alpha(\Gamma, x) = (3q-1)px^{9^\alpha} + 2px^{6^\alpha} + px^{4^\alpha}.$$

For $\alpha = 1$ the second Zagreb polynomial is

$$R_1(\Gamma, x) = (3q-1)px^9 + 2px^6 + px^4.$$

For $X_\alpha(\Gamma, x)$ that is the general sum-connectivity polynomial we have $g(d_v, d_u) = (d_v + d_u)^\alpha$, thus $g(3,3) = 6^\alpha$, $g(3,2) = 5^\alpha$ and $g(2,2) = 4^\alpha$. Hence by Theorem 3.1,

$$X_\alpha(\Gamma, x) = (3q-1)px^{6^\alpha} + 2px^{5^\alpha} + px^{4^\alpha}.$$

For $\alpha = 1$ the first Zagreb polynomial is

$$X_1(\Gamma, x) = (3q-1)px^6 + 2px^5 + px^4.$$

For $\alpha = 2$ the hyper-Zagreb polynomial is

$$X_2(\Gamma, x) = (3q-1)px^{36} + 2px^{25} + px^{16}.$$

For $GZ(\Gamma, x)$ which is the generalized Zagreb polynomial we have $g(d_v, d_u) = d_v^\alpha d_u^\beta + d_u^\alpha d_v^\beta$, so $g(3,3) = 2 \cdot 3^\alpha 3^\beta = 2 \cdot 3^{\alpha+\beta}$, $g(3,2) = 2^\alpha 3^\beta + 3^\alpha 2^\beta$ and $g(2,2) = 2 \cdot 2^\alpha 2^\beta = 2^{\alpha+\beta+1}$. Thus

$$GZ_{\alpha,\beta}(\Gamma, x) = (3q-1)px^{2\cdot 3^{\alpha+\beta}} + 2px^{2^\alpha 3^\beta + 3^\alpha 2^\beta} + px^{2^{\alpha+\beta+1}}.$$

If $\alpha = 2$ and $\beta = 0$, we get the forgotten polynomial

$$GZ_{2,0}(\Gamma, x) = (3q-1)px^{18} + 2px^{13} + px^8.$$

For the third redefined Zagreb polynomial $ReZ(\Gamma, x)$ we have $g(d_v, d_u) = d_v d_u(d_v + d_u)$, thus $g(3,3) = 54$, $g(3,2) = 30$ and $g(2,2) = 16$. Hence

$$ReZ(\Gamma, x) = (3q-1)px^{54} + 2px^{30} + px^{16}.$$

For the harmonic polynomial of Γ we have $g(d_v, d_u) = d_v + d_u - 1$, thus $g(3,3) = 5$, $g(3,2) = 4$ and $g(2,2) = 3$. Hence

$$H(\Gamma, x) = 2[(3q-1)px^5 + 2px^4 + px^3] = (3q-1)2px^5 + 4px^4 + 2px^3.$$

□

4. **Zig-zag polyhex nanotubes**

Let us investigate zig-zag polyhex nanotubes $TUZC_6[p;q]$. The number of hexagons in every column of the corresponding two-dimensional lattice is $p \geq 2$ the number of hexagons in every row is $q \geq 1$; see Figure 2.

We give a general formula and use it to obtain any polynomial of topological indices based on degrees for zig-zag polyhex nanotubes.

Theorem 4.1. *For the zig-zag polyhex nanotube* $\Gamma = TUZC_6[p;q]$, *we have*

$$P(\Gamma, x) = \sum_{vu \in E(\Gamma)} x^{g(d_v, d_u)} = (3q-2)p \cdot x^{g(3,3)} + 4p \cdot x^{g(3,2)}.$$

Proof. The nanotube $TUZC_6[p;q]$ contains $(q+1)2p$ vertices and $(3q+2)p$ edges. Any vertex has degree either two or three. $V(\Gamma)$ can be divided into the sets:

$$V_2 = \{u \in V(\Gamma) \mid d_u = 2\} \quad \text{and} \quad V_3 = \{u \in V(\Gamma) \mid d_u = 3\}.$$

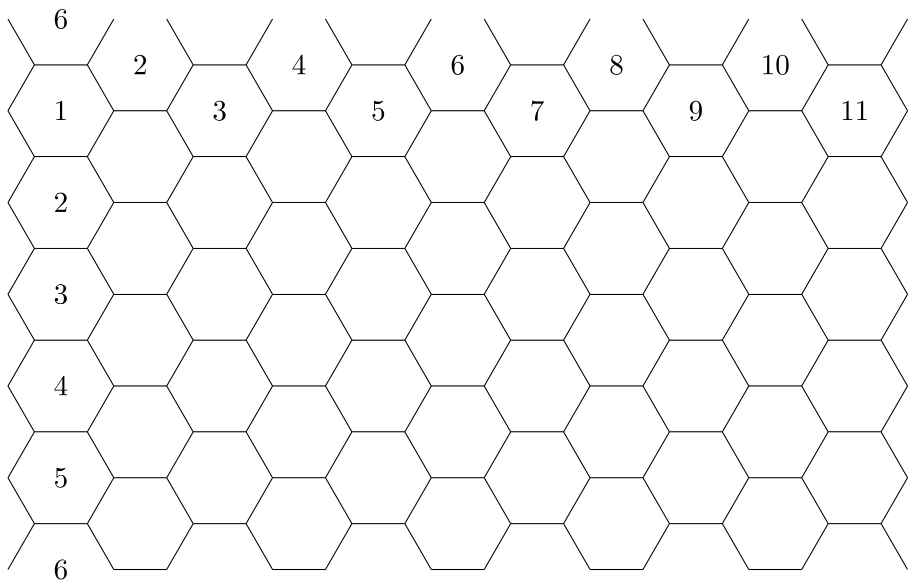

Fig. 2. Zig-zag polyhex nanotube $TUZC_6[p;q]$ for $p = 6$ and $q = 11$

We have $|V_2| = 2p$ and $|V_3| = 2qp$. Let

$$\begin{aligned} E_{3,2} &= \{vu \in E(\Gamma) \mid d_v = 3,\ d_u = 2\}, \\ E_{3,3} &= \{vu \in E(\Gamma) \mid d_v = d_u = 3\}. \end{aligned}$$

Note that $E(\Gamma) = E_{3,2} \cup E_{3,3}$. Each vertex having degree two is adjacent to two vertices having degree three, thus we get $|E_{3,2}| = 4p$. Then $|E_{3,3}| = |E(\Gamma)| - |E_{3,2}| = (3q-2)p$ and

$$\begin{aligned} P(\Gamma, x) &= \sum_{vu \in E(\Gamma)} x^{g(d_v,d_u)} = \sum_{vu \in E_{3,3}} x^{g(3,3)} + \sum_{vu \in E_{3,2}} x^{g(3,2)} \\ &= (3q-2)p \cdot x^{g(3,3)} + 4p \cdot x^{g(3,2)}. \end{aligned}$$

□

Now we present the best-known polynomials for zig-zag polyhex nanotubes.

Corollary 4.1. *For the zig-zag polyhex nanotube $\Gamma = TUZC_6[p;q]$, the general Randić polynomial of Γ is*

$$R_\alpha(\Gamma, x) = (3q-2)px^{9^\alpha} + 4px^{6^\alpha},$$

the second Zagreb polynomial

$$R_1(\Gamma, x) = (3q-2)px^9 + 4px^6,$$

the general sum-connectivity polynomial

$$X_\alpha(\Gamma, x) = (3q-2)px^{6^\alpha} + 4px^{5^\alpha},$$

the first Zagreb polynomial

$$X_1(\Gamma, x) = (3q-2)px^6 + 4px^5,$$

the hyper-Zagreb polynomial

$$X_2(\Gamma, x) = (3q-2)px^{36} + 4px^{25},$$

the generalized Zagreb polynomial

$$GZ_{\alpha,\beta}(\Gamma, x) = (3q-2)px^{2\cdot 3^{\alpha+\beta}} + 4px^{2^\alpha 3^\beta + 3^\alpha 2^\beta},$$

the forgotten polynomial

$$GZ_{2,0}(\Gamma, x) = (3q-2)px^{18} + 4px^{13},$$

the third redefined Zagreb polynomial

$$ReZ(\Gamma, x) = (3q-2)px^{54} + 4px^{30}$$

and the harmonic polynomial

$$H(\Gamma, x) = (3q-2)2px^5 + 8px^4.$$

Proof. For $R_\alpha(\Gamma, x)$ which is the general Randić polynomial, we get $g(d_v, d_u) = (d_v d_u)^\alpha$, so $g(3,3) = 9^\alpha$ and $g(3,2) = 6^\alpha$. From Theorem 4.1,

$$R_\alpha(\Gamma, x) = (3q-2)px^{9^\alpha} + 4px^{6^\alpha}.$$

For $\alpha = 1$ the second Zagreb polynomial is

$$R_1(\Gamma, x) = (3q-2)px^9 + 4px^6.$$

For $X_\alpha(\Gamma, x)$ that is the general sum-connectivity polynomial, we have $g(d_v, d_u) = (d_v + d_u)^\alpha$, therefore $g(3,3) = 6^\alpha$ and $g(3,2) = 5^\alpha$. From Theorem 4.1,

$$X_\alpha(\Gamma, x) = (3q-2)px^{6^\alpha} + 4px^{5^\alpha}.$$

For $\alpha = 1$ the first Zagreb polynomial is

$$X_1(\Gamma, x) = (3q-2)px^6 + 4px^5.$$

For $\alpha = 2$ the hyper-Zagreb polynomial is

$$X_2(\Gamma, x) = (3q-2)px^{36} + 4px^{25}.$$

For $GZ(\Gamma, x)$ which is the generalized Zagreb polynomial, we obtain $g(d_v, d_u) = d_v^\alpha d_u^\beta + d_u^\alpha d_v^\beta$, so $g(3,3) = 2\cdot 3^\alpha 3^\beta = 2\cdot 3^{\alpha+\beta}$ and $g(3,2) = 2^\alpha 3^\beta + 3^\alpha 2^\beta$. Thus

$$GZ_{\alpha,\beta}(\Gamma, x) = (3q-2)px^{2\cdot 3^{\alpha+\beta}} + 4px^{2^\alpha 3^\beta + 3^\alpha 2^\beta}.$$

If $\alpha = 2$ and $\beta = 0$, we get the forgotten polynomial

$$GZ_{2,0}(\Gamma, x) = (3q-2)px^{18} + 4px^{13}.$$

For the third redefined Zagreb polynomial $ReZ(\Gamma, x)$ we have $g(d_v, d_u) = d_v d_u (d_v + d_u)$, thus $g(3,3) = 54$ and $g(3,2) = 30$. Hence

$$ReZ(\Gamma, x) = (3q-2)px^{54} + 4px^{30}.$$

For the harmonic polynomial of Γ we have $g(d_v, d_u) = d_v + d_u - 1$, thus $g(3,3) = 5$ and $g(3,2) = 4$. Hence

$$H(\Gamma, x) = 2[(3q-2)px^5 + 4px^4] = (3q-2)2px^5 + 8px^4.$$

□

Let us show that the derivatives of polynomials can be easily applied to obtain the values of topological indices for hexagonal nanotubes (when using $x = 1$ in the derivative). For the armchair polyhex nanotube $\Gamma = TUAC_6[p;q]$, we have

$$P'(\Gamma, x) = (3q-1)p \cdot g(3,3)x^{g(3,3)-1} + 2p \cdot g(3,2)x^{g(3,2)-1} + p \cdot g(2,2)x^{g(2,2)-1},$$

therefore the general expression of a topological index of the armchair polyhex nanotube is

$$P'(\Gamma, 1) = (3q-1)p \cdot g(3,3) + 2p \cdot g(3,2) + p \cdot g(2,2).$$

For the zig-zag polyhex nanotube $\Gamma = TUZC_6[p;q]$, we have

$$P'(\Gamma, x) = (3q-2)p \cdot g(3,3)x^{g(3,3)-1} + 4p \cdot g(3,2)x^{g(3,2)-1},$$

therefore the general expression of a topological index of $\Gamma = TUZC_6[p;q]$ is

$$P'(\Gamma, 1) = (3q-2)p \cdot g(3,3) + 4p \cdot g(3,2).$$

For example, for the general Randić polynomial we have $g(d_v, d_u) = (d_v d_u)^\alpha$ which implies that $g(3,3) = 9^\alpha$, $g(3,2) = 6^\alpha$ and $g(2,2) = 4^\alpha$. Thus the general Randić index of the armchair polyhex nanotube is

$$R'_\alpha(\Gamma, 1) = (3q-1)p \cdot 9^\alpha + 2p \cdot 6^\alpha + p \cdot 4^\alpha.$$

For the general Randić polynomial of the zig-zag polyhex nanotube $\Gamma = TUZC_6[p;q]$ we have $g(3,3) = 9^\alpha$ and $g(3,2) = 6^\alpha$. thus the general Randić index of the zig-zag polyhex nanotube is

$$R'_\alpha(\Gamma, 1) = (3q-2)p \cdot 9^\alpha + 4p \cdot 6^\alpha.$$

Similarly, we can use polynomials to obtain other topological indices.

5. **Summary of results**

In Theorem 3.1 and Corollary 3.1 we stated that for the armchair polyhex nanotube $\Gamma = TUAC_6[p;q]$, we have

$$\begin{aligned}
P(\Gamma,x) &= \sum_{vu\in E(\Gamma)} x^{g(d_v,d_u)} = (3q-1)p\cdot x^{g(3,3)} + 2p\cdot x^{g(3,2)} + p\cdot x^{g(2,2)}.\\
R_\alpha(\Gamma,x) &= (3q-1)px^{9^\alpha} + 2px^{6^\alpha} + px^{4^\alpha},\\
R_1(\Gamma,x) &= (3q-1)px^9 + 2px^6 + px^4,\\
X_\alpha(\Gamma,x) &= (3q-1)px^{6^\alpha} + 2px^{5^\alpha} + px^{4^\alpha},\\
X_1(\Gamma,x) &= (3q-1)px^6 + 2px^5 + px^4,\\
X_2(\Gamma,x) &= (3q-1)px^{36} + 2px^{25} + px^{16},\\
GZ_{\alpha,\beta}(\Gamma,x) &= (3q-1)px^{2\cdot 3^{\alpha+\beta}} + 2px^{2^\alpha 3^\beta + 3^\alpha 2^\beta} + px^{2^{\alpha+\beta+1}},\\
GZ_{2,0}(\Gamma,x) &= (3q-1)px^{18} + 2px^{13} + px^8,\\
ReZ(\Gamma,x) &= (3q-1)px^{54} + 2px^{30} + px^{16},\\
H(\Gamma,x) &= (3q-1)2px^5 + 4px^4 + 2px^3.
\end{aligned}$$

Theorem 4.1 and Corollary 4.1 say that for the zig-zag polyhex nanotube $\Gamma = TUZC_6[p;q]$, we have

$$\begin{aligned}
P(\Gamma,x) &= \sum_{vu\in E(\Gamma)} x^{g(d_v,d_u)} = (3q-2)p\cdot x^{g(3,3)} + 4p\cdot x^{g(3,2)},\\
R_\alpha(\Gamma,x) &= (3q-2)px^{9^\alpha} + 4px^{6^\alpha},\\
R_1(\Gamma,x) &= (3q-2)px^9 + 4px^6,\\
X_\alpha(\Gamma,x) &= (3q-2)px^{6^\alpha} + 4px^{5^\alpha},\\
X_1(\Gamma,x) &= (3q-2)px^6 + 4px^5,\\
X_2(\Gamma,x) &= (3q-2)px^{36} + 4px^{25},\\
GZ_{\alpha,\beta}(\Gamma,x) &= (3q-2)px^{2\cdot 3^{\alpha+\beta}} + 4px^{2^\alpha 3^\beta + 3^\alpha 2^\beta},\\
GZ_{2,0}(\Gamma,x) &= (3q-2)px^{18} + 4px^{13},\\
ReZ(\Gamma,x) &= (3q-2)px^{54} + 4px^{30},\\
H(\Gamma,x) &= (3q-2)2px^5 + 8px^4.
\end{aligned}$$

6. **Conclusion**

Topological indices are extensively used for establishing relationships between the structure of nanotubes and their physico-chemical properties. These indices are a convenient method of translating chemical constitution into numerical values which are used for correlations with physical properties.

There are two types of hexagonal nanotubes: armchair polyhex nanotubes and zig-zag polyhex nanotubes; see Figures 1 and 2. We can represent these nanotubes by graphs that consist of vertices and edges.

Topological indices are often studied with the help of their polynomials. In this paper we presented general formulas and used them to obtain any polynomial of degree-based indices for hexagonal nanotubes. We showed that the derivatives of these polynomials can be used to obtain various topological indices such as the general Randić index for hexagonal nanotubes.

7. Notations

Γ	graph
$E(\Gamma)$	edge set of a graph
$V(\Gamma)$	vertex set of a graph
d_u	degree of a vertex u – the number of neighbours of u
V_i	set containing vertices of degree i
$E_{i,j}$	set containing edges with one vertex having degree i and the other vertex having degree j
$\lvert E_{i,j}\rvert$	the number of edges in $E_{i,j}$
vu	edge containing vertices v and u
$g(d_v, d_u)$	function of d_v and d_u which depends on a particular topological index
$P(\Gamma, x)$	general polynomial
$TUAC_6[p;q]$	armchair polyhex nanotube
$TUZC_6[p;q]$	zig-zag polyhex nanotube
$P(\Gamma, x)$	general polynomial of Γ which is used to study all the other polynomials
$R_\alpha(\Gamma, x)$	general Randić polynomial of Γ
$R_1(\Gamma, x)$	second Zagreb polynomial
$X_\alpha(\Gamma, x)$	general sum-connectivity polynomial
$X_1(\Gamma, x)$	first Zagreb polynomial
$X_2(\Gamma, x)$	hyper-Zagreb polynomial
$GZ_{\alpha,\beta}(\Gamma, x)$	generalized Zagreb polynomial
$GZ_{2,0}(\Gamma, x)$	forgotten polynomial
$ReZ(\Gamma, x)$	third redefined Zagreb polynomial
$H(\Gamma, x)$	harmonic polynomial

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