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Research Article

Analysis of $SC_5C_7[p, q]$ and $NPHX[p, q]$ Nanotubes via Topological Indices

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Scientists are creating materials, for example, a carbon nanotube-based composite created by NASA that bends when a voltage is connected. Applications incorporate the use of an electrical voltage to change the shape (transform) of air ship wings and different structures. Topological indices are numbers related with molecular graphs to allow quantitative structure activity/property/poisonous relationships. Topological indices catch symmetry of molecular structures and give it a scientific dialect to foresee properties, for example, boiling points, viscosity, and the radius of gyrations. We compute M-polynomials of two nanotubes, $SC_5C_7[p, q]$ and $NPHX[p, q]$. The closed form of M-polynomials for these nanotubes produces formulas of numerous degree-based topological indices which are functions relying on parameters of the structure and, in combination, decide properties of the concerned nanotubes. Moreover, we sketch our results by using Maple 2015 to see the dependence of our results on the involved parameters.

1. Introduction

The expression "nano" alludes to the metric prefix 10^{-9}. It implies one billionth of something. "Nano" can be attributed to any unit of measure. For instance, you may report a little mass in nanograms or the measure of fluid in one cell as far as nanoliters. Nanoscience is the investigation of structures and materials on the size of nanometers. When structures are made enough in the nanometer measure range, they can go up against fascinating and valuable properties. Nanoscale structures have existed in nature well before researchers started considering them in labs. Researchers have even made nanostructures in the lab that copy a portion of nature's stunning nanostructures [1–3].

Nanoscience has effectively affected our lives with developments, for example, stain-resistant fabrics propelled by nanoscale highlights found on lotus plants and PC hard drives, which store data on magnetic strips that are only 20 nanometers thick. Researchers from several disciplines material science, biology, chemistry, and physics utilize nanoscience standards for applications in computing, medication, energy, information storage, etc. In spite of the fact that achievements in any research field are hard to anticipate, the eventual fate of nanoscience will probably include scaling up from atomic get together and singular nanodevices to macroscopic systems and structures with developing properties and different capacities. Carbon nanotubes can be utilized as the pores in layers to run reverse osmosis desalination plants. Water atoms go through the smoother walls of carbon nanotubes more effortlessly than through different sorts of nanopores, which requires less power. Different scientists are utilizing carbon nanotubes to develop little, inexpensive water purification devices required in poor nations. Sensors utilizing carbon nanotube detection elements are fit

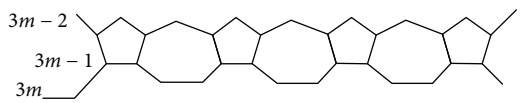

Figure 1: ith period of $SC_5C_7[p, q]$ nanotube.

for distinguishing a scope of chemical vapors. These sensors work by responding to the changes in the resistance of a carbon nanotube within the sight of a chemical vapor [4–7].

The features of energetics and electronic properties of carbon nanotubes, containing a pentagon-heptagon pair (5/7) topological defect in the hexagonal network of the zigzag configuration, are investigated using the extended Su-Schriffer-Heeger model based on the tight binding approximation in real space. Calculations show that this pentagon-heptagon pair defect in the nanotube structures is not only responsible for a change in nanotube diameter but also governs the electronic behavior around the Fermi level [8].

In nanoscience, $SC_5C_7[p, q]$ (where p and q express the number of heptagons in each row and the number of periods in whole lattice, respectively) nanotube is a class of C_5C_7 net which is yielded by alternating C_5 and C_7. The standard tiling of C_5 and C_7 can cover either a cylinder or a torus, and each period of $SC_5C_7[p, q]$ consisted of three rows (more details on pth period can be referred to in Figure 1). H-Naphtalenic nanotubes $NPHX[p, q]$ (where p and q are denoted as the number of pairs of hexagons in first row and the number of alternative hexagons in a column, respectively) are a trivalent decoration with sequence of C_6, C_6, C_4, C_6, C_6, C_4, … in the first row and a sequence of C_6, C_8, C_6, C_8, … in the other rows. In other words, this nanolattice can be considered as a plane tiling of C_4, C_6, and C_8. Therefore, this class of tiling can cover either a cylinder or a torus [9].

In the field of chemical graph theory, the molecular graph G is a simple connected graph in which atoms are taken as vertices and chemical bonds are taken as edges. The vertex set is usually denoted by V, and the edge set is denoted by E. The degree of a vertex v is denoted by d_v, which is the total number of vertices attached with it. The valence in chemistry and the degree of a vertex in a graph are closely related. For details about graph theory and its notion, we refer to the book [10].

Another emerging field is cheminformatics. In cheminformatics, the quantitative structure-activity (QSAR) and the structure-property (QSPR) relationship foresees the biological activity and properties of understudy nanomaterial. In these investigations, topological indices and some physicochemical properties are utilized to foresee bioactivity of understudy nanomaterial, see [11–15]. Polynomials have additionally valuable applications in chemical graph theory, for example, Hosoya polynomial (also called Wiener polynomial) [16] which assumes an indispensable job in deciding distance-based topological indices. Among other polynomials, M-polynomial [17] presented in 2015 assumes a similar job in deciding the closed form of many degree-based topological indices [18–22]. The primary favorable position of M-polynomial is the abundance of data that it contains about degree-based graph invariants.

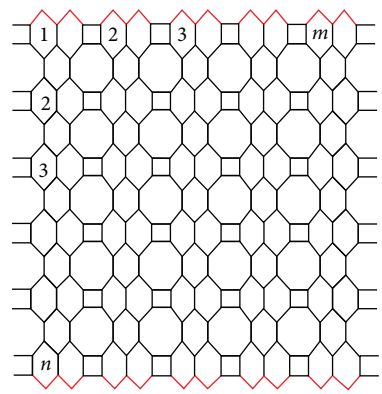

Figure 2: Naphtalenic nanotubes.

In this paper, we focus on the degree-based combinatorial facts of two nanotubes. At first, we give M-polynomial of these nanotubes shown in Figures 1 and 2. Then, by using calculus rules on the M-polynomials, we recover nine topological indices.

2. Basic Definition and Literature Review

In this section, we give basic definitions and notions. Throughout this paper, we fix the following notion.

(1) G = connected simple graph

(2) $V(G)$ = set of vertices of G

(3) $E(G)$ = set of edges

(4) $|V(G)|$ = numbers of elements in $V(G)$

(5) $|E(G)|$ = numbers of elements in $E(G)$

(6) d_v = degree of vertex v

Definition 1 (see [17]). For a simple connected graph G, the M-polynomial is defined as follows:

$$M(G; x, y) = \sum_{\delta \le i \le j \le \Delta} m_{ij}(G) x^i y^j, \tag{1}$$

where $\Delta = \mathrm{Min}\{d_v : v \in V(G)\}$, $\Delta = \mathrm{Max}\{d_v : v \in V(G)\}$, and $m_{ij}(G)$ is the edge $vu \in E(G)$ such that $\{d_v, d_u\} = \{i, j\}$.

In 1947, the first topological index was introduced by Wiener, when he was studying the boiling point of alkanes [23]. Subsequently, Wiener established the framework of the topological index [24, 25].

After Wiener, in 1975, Milan Randić introduced the Randić index $R_{-1/2}(G)$ in [26], which is defined as

$$R_{-1/2}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}, \tag{2}$$

and is one of the oldest degree-based topological index. In the year 1998, researchers in [27, 28] introduced the generalized version of the Randić index. The generalized Randić index gets a great attention from a mathematician [29]. We refer to [30] for mathematical properties of this index, and for detailed survey, we refer to [31]. The general Randić index is defined as

$$R_\alpha(G) = \sum_{uv\in E(G)} \frac{1}{(d_u d_v)^\alpha}, \tag{3}$$

and the generalized inverse Randić index is defined as

$$RR_\alpha(G) = \sum_{uv\in E(G)} (d_u d_v)^\alpha. \tag{4}$$

If we take $\alpha = -1/2$ in the generalized Randić index, we get $R_{-1/2}(G)$. The Randić index is likewise the most mainstream regularly connected and most concentrated among all other topological indices. Numerous papers and books, for example, [32–34], are written on this topological index. Randić himself wrote two surveys on his Randić index [35, 36], and there are three more surveys [37–39].

The first and second Zagreb indices are defined by Gutman et al. as

$$\begin{aligned} M_1(G) &= \sum_{uv\in E(G)} (d_u + d_v), \\ M_2(G) &= \sum_{uv\in E(G)} (d_u \times d_v). \end{aligned} \tag{5}$$

For insight about these indices, we refer [40–44] to the readers. Both the first Zagreb index and the second Zagreb index give more weights to the internal vertices and edges and less weights to external vertices and edges which contradict instinctive thinking. Consequently, they were modified in [45] as the second modified Zagreb index:

$${}^mM_2(G) = \sum_{uv\in E(G)} \frac{1}{d(u)d(v)}. \tag{6}$$

The symmetric division index (SDD) is one of the 148 discrete Adriatic indices and is a decent indicator of the aggregate surface area for polychlorobiphenyls [46]. The symmetric division index of a graph G is defined as

$$\mathrm{SDD}(G) = \sum_{uv\in E(G)} \left\{ \frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)} \right\}. \tag{7}$$

Harmonic index is defined as

$$H(G) = \sum_{vu\in E(G)} \frac{2}{d_u + d_v}. \tag{8}$$

As far as we know, this index firstly appeared in [47] and studied in [48].

Table 1

Topological index	Derivation from $M(G;x,y)$
M_1	$(D_x + D_y)(M(G;x,y))_{x=y=1}$
M_2	$(D_x D_y)(M(G;x,y))_{x=y=1}$
${}^mM_2$	$(S_x S_y)(M(G;x,y))_{x=y=1}$
R_α	$(D_x^\alpha D_y^\alpha)(M(G;x,y))_{x=y=1}$
RR_α	$(S_x^\alpha S_y^\alpha)(M(G;x,y))_{x=y=1}$
SSD	$(D_x S_y + S_x D_y)(M(G;x,y))_{x=y=1}$
H	$2S_x J(M(G;x,y))_{x=1}$
I	$S_x J D_x D_y (M(G;x,y))_{x=1}$
A	$S_x{}^3 Q_{-2} J D_x{}^3 D_y{}^3 (M(G;x,y))_{x=1}$

$D_x = x(\partial(f(x,y))/\partial x)$, $D_y = y(\partial(f(x,y))/\partial y)$, $S_x = \int_0^x (f(t,y)/t)dt$, $S_y = \int_0^y (f(x,t)/t)dt$, $J(f(x,y)) = f(x,x)$, and $Q_\alpha(f(x,y)) = x^\alpha f(x,y)$.

The inverse sum index is the descriptor that was chosen in [49] as a huge indicator of the aggregate surface area of octane isomers and for which the extremal graphs acquired have an especially straightforward and rich structure. It is denoted by I and is defined as

$$I(G) = \sum_{vu\in E(G)} \frac{d_u d_v}{d_u + d_v}. \tag{9}$$

In [50], Furtula et al. defined the augmented Zagreb index as

$$A(G) = \sum_{vu\in E(G)} \left\{ \frac{d_u d_v}{d_u + d_v - 2} \right\}^3. \tag{10}$$

This graph invariant has wound up being a critical judicious index in the examination of the heat formation in heptanes and octanes (see [50]), whose forecast control is better than the atomic bond connectivity (ABC) index [51–53]. The relationship between M-polynomial and indices is presented in Table 1 [17].

3. Main Results

In this section, we give our computational results.

3.1. M-Polynomial and Degree-Based Topological Indices of $\mathrm{SC_5C_7}[p,q]$

Theorem 1. *The M-polynomial of* $\mathrm{SC_5C_7}[p,q]$ *nanotube is*

$$M(\mathrm{SC_5C_7}[p,q], x, y) = px^2y^2 + [12pq - 9p]x^3y^3 + 6px^2y^3. \tag{11}$$

Proof 1. Then, the vertex set of $\mathrm{SC_5C_7}[p,q]$ has the following two partitions with respect to degree:

$$V_{\{2\}}(SC_5C_7[p,q]) = \left\{v \in V(SC_5C_7[p,q])|_{d_v=2}\right\},$$
$$V_{\{3\}}(SC_5C_7[p,q]) = \left\{v \in V(SC_5C_7[p,q])|_{d_v=3}\right\}. \quad (12)$$

The edge set of $SC_5C_7[p,q]$ has three partitions based on the degree of end vertices:

$$E_{\{2,2\}}(SC_5C_7[p,q]) = \left\{e = uv \in E(SC_5C_7[p,q])|_{d_u=2,d_v=2}\right\},$$
$$E_{\{3,3\}}(SC_5C_7[p,q]) = \left\{e = uv \in E(SC_5C_7[m,n])|_{d_u=3,d_v=3}\right\},$$
$$E_{\{2,3\}}(SC_5C_7[p,q]) = \left\{e = uv \in E(SC_5C_7[p,q])|_{d_u=2,d_v=3}\right\}, \quad (13)$$

such that

$$\left|E_{\{2,2\}}(SC_5C_7[p,q])\right| = p,$$
$$\left|E_{\{3,3\}}(SC_5C_7[p,q])\right| = 12pq - 9p, \quad (14)$$
$$\left|E_{\{2,3\}}(SC_5C_7[p,q])\right| = 6p.$$

Now,

$$\begin{aligned}
M(SC_5C_7[p,q],x,y) &= \sum_{i\leq j} m_{ij}(SC_5C_7[p,q])x^iy^j \\
&= \sum_{2\leq 2} m_{22}(SC_5C_7[p,q])x^2y^2 \\
&\quad + \sum_{3\leq 3} m33(SC_5C_7[p,q])x^3y^3 \\
&\quad + \sum_{2\leq 3} m_{23}(SC_2C_3[p,q])x^2y^3 \\
&= \sum_{uv\in E_{\{2,2\}}(SC_5C_7[p,q])} m_{22}(SC_5C_7[p,q])x^2y^2 \\
&\quad + \sum_{uv\in E_{\{3,3\}}(SC_5C_7[p,q])} m_{33}(SC_5C_7[p,q])x^3y^3 \\
&\quad + \sum_{uv\in E_{\{2,3\}}(SC_5C_7[p,q])} m_{23}(SC_5C_7[p,q])x^2 \\
&= \left|E_{\{2,2\}}(SC_5C_7[p,q])\right|x^2y^2 \\
&\quad + \left|E_{\{3,3\}}(SC_5C_7[p,q])\right|x^3y^3 \\
&\quad + \left|E_{\{2,3\}}(SC_5C_7[p,q])\right|x^2y^3 \\
&= px^2y^2 + [12pq - 9p]x^3y^3 + 6px^2y^3.
\end{aligned} \quad (15)$$

Figure 3 shows the behavior of M-polynomial of $SC_5C_7[p,q]$ onto the involved parameters x, y.

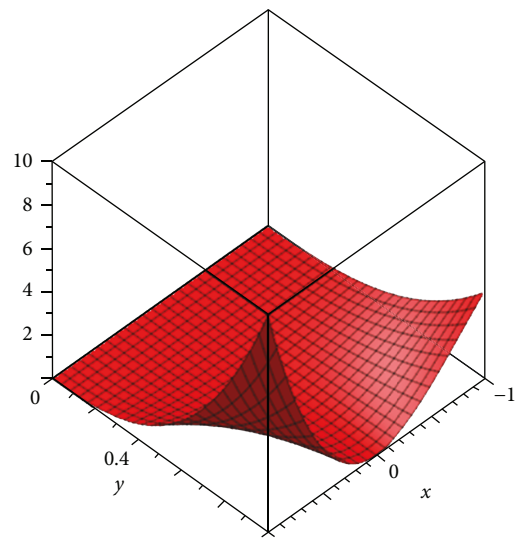

Figure 3: Plot of M-polynomial of $SC_5C_7[1,1]$.

Proposition 2. *For the nanotube* $SC_5C_7[p,q]$, *we have*

$$\begin{aligned}
M_1(SC_5C_7[p,q]) &= 72pq - 20p, \\
M_2(SC_5C_7[p,q]) &= 108pq - 41p, \\
{}^mM_2(SC_5C_7[p,q]) &= \frac{4}{3}pq + \frac{1}{4}p, \\
R_\alpha(SC_5C_7[p,q]) &= 2^{2\alpha}p + (12pq - 9p)3^{2\alpha} - 3^\alpha 2^\alpha 6p, \\
RR_\alpha(SC_5C_7[p,q]) &= \frac{p}{2^{2\alpha}} + \frac{12}{3^{2\alpha}}pq - \frac{9}{3^{2\alpha}}p + \frac{6}{3^\alpha \cdot 2^\alpha}p, \\
SSD(SC_5C_7[p,q]) &= 24pq - 5p, \\
H(SC_5C_7[p,q]) &= 4pq - \frac{1}{10}p, \\
I(SC_5C_7[p,q]) &= 18pq - \frac{53}{10}p, \\
A(SC_5C_7[p,q]) &= \frac{47}{8}p + \frac{27}{2}pq.
\end{aligned} \quad (16)$$

Proof 2. Let

$$\begin{aligned}
M(SC_5C_7[p,q];x,y) = f(x,y) &= px^2y^2 + 6px^2y^3 \\
&\quad + (12pq - 9p)x^3y^3.
\end{aligned} \quad (17)$$

Then,

$$\begin{aligned}
D_yf(x,y) &= 2px^2y^2 + 18px^2y^3 + 3(12pq - 9p)x^3y^3, \\
D_xf(x,y) &= 2px^2y^2 + 12px^2y^3 + 3(12pq - 9p)x^3y^3, \\
D_yD_xf(x,y) &= 4px^2y^2 + 36px^2y^3 + 9(12pq - 9p)x^2y^3, \\
S_xS_y(f(x,y) &= \frac{1}{4}px^2y^2 + px^2y^3 + \frac{1}{9}(12pq - 9p)x^3y^3, \\
D_x^aD_y^a(f(x,y) &= 2^{2\alpha}px^2y^2 + 2^\alpha 3^\alpha 6px^2y^3 + 3^{2\alpha}(12pq - 9p)x^3y^3,
\end{aligned}$$

$$\begin{aligned}
S_x^a S_y^a(f(x,y)) &= \frac{1}{2^{2\alpha}}px^2y^2 + \frac{6}{2^\alpha 3^\alpha}px^2y^3 + \frac{1}{3^{2\alpha}}(12pq-9p)x^3y^3,\\
S_yD_x(f(x,y)) &= px^2y^2 + \frac{12}{3}px^2y^3 + (12pq-9p)x^3y^3,\\
S_xD_y(f(x,y)) &= px^2y^2 + 9px^2y^3 + (12pq-9p)x^3y^3,\\
2S_xJf(x,y) &= 2\left[px^6 + \frac{6}{5}px^5 + (12pq-9p)x^6\right],\\
S_x^3Q_{-2}JD_x^3D_y^3f(x,y) &= \frac{47}{8}p + \frac{27}{2}pq.
\end{aligned} \tag{18}$$

Now from Table 1,

(1) First Zagreb index

$$\begin{aligned}
M_1(G) &= (D_x + D_y)f(x,y)\big|_{x=y=1}\\
&= 14p + 6(12pq-9p) + 30p
\end{aligned} \tag{19}$$

(2) Second Zagreb index

$$\begin{aligned}
M_2(G) &= D_yD_x(f(x,y))\big|_{x=y=1}\\
&= 4p + 9(12pq-9p) + 36p
\end{aligned} \tag{20}$$

(3) Modified second Zagreb index

$$\begin{aligned}
{}^mM_2(G) &= S_xS_y(f(x,y))\big|_{x=y=1}\\
&= \frac{1}{4}p + \frac{1}{9}(12pq-9p) + p
\end{aligned} \tag{21}$$

(4) Generalized Randić index

$$\begin{aligned}
R_\alpha(G) &= D_x^\alpha D_y^\alpha(f(x,y))\Big|_{x=y=1}\\
&= 2^{2\alpha}p + 3^{2\alpha}(12pq-9p) + 2^\alpha\cdot 3^\alpha(6p)
\end{aligned} \tag{22}$$

(5) Inverse Randić index

$$\begin{aligned}
RR_\alpha(G) &= S_x^\alpha S_y^\alpha(f(x,y))\Big|_{x=y=1}\\
&= \frac{1}{2^{2\alpha}}p + \frac{2}{3^{2\alpha}}(12pq-9p) + \frac{1}{2^\alpha\cdot 3^\alpha}6p
\end{aligned} \tag{23}$$

(6) Symmetric division index

$$\begin{aligned}
\mathrm{SSD}(G) &= (S_yD_x + S_xD_y)(f(x,y))\big|_{x=y=1}\\
&= 2p + 2(24pq-9p) + 4p + 9p
\end{aligned} \tag{24}$$

(7) Harmonic index

$$H(G) = 2S_xJ(f(x,y))\big|_{x=1} = \frac{1}{4}p + \frac{1}{6}(12pq-9p) + \frac{6}{5}p \tag{25}$$

(8) Inverse sum index

$$I(G) = S_xJD_xD_y(f(x,y))_{x=1} = p + \frac{3}{2}(12pq-9p) + \frac{36}{5}p \tag{26}$$

(9) Augmented Zagreb index

$$A(G) = S_x{}^3Q_{-2}JD_x{}^3D_y{}^3f(x,y) = \frac{47}{8}p + \frac{27}{2}pq \tag{27}$$

3.2. The M-Polynomial and Degree-Based Topological Indices of NPHX[p, q]

Theorem 3. *For the H-naphtalenic nanotubes* NPHX[p, q], *we have*

$$M(\mathrm{NPHX}[m,n],x,y) = (15mn-10m)x^3y^3 + 8mx^2y^3. \tag{28}$$

Proof 3. The edge set of NPHX[p, q] has the following two partitions with respect to degree of the end vertices:

$$\begin{aligned}
E_{\{3,3\}} &= \left\{e = uv \in E(\mathrm{NPHX}[p,q])\big|_{d_u=3,d_v=3}\right\},\\
E_{\{2,3\}} &= \left\{e = uv \in E(\mathrm{NPHX}[p,q])\big|_{d_u=2,d_v=3}\right\},
\end{aligned} \tag{29}$$

such that

$$\begin{aligned}
\left|E_{\{3,3\}}\right| &= 15pq - 10p,\\
\left|E_{\{2,3\}}\right| &= 8p.
\end{aligned} \tag{30}$$

Now,

$$\begin{aligned}
M(\mathrm{NPHX}[p,q],x,y) &= \sum_{i\le j} m_{ij}(\mathrm{NPHX}[p,q]x^iy^j)\\
&= \sum_{3\le 3} m_{33}(\mathrm{NPHX}[p,q])x^3y^3\\
&\quad + \sum_{2\le 3} m_{23}(\mathrm{NPHX}[p,q])x^2y^3\\
&= \sum_{uv\in E_{\{3,3\}}} m_{33}(\mathrm{NPHX}[p,q])x^3y^3\\
&\quad + \sum_{uv\in E_{\{2,3\}}} m_{23}(\mathrm{NPHX}[p,q])x^2y^3\\
&= \left|E_{\{3,3\}}\right|x^3y^3 + \left|E_{\{2,3\}}\right|x^2y^3\\
&= [15pq-10p]x^3y^3 + 8px^2y^3.
\end{aligned} \tag{31}$$

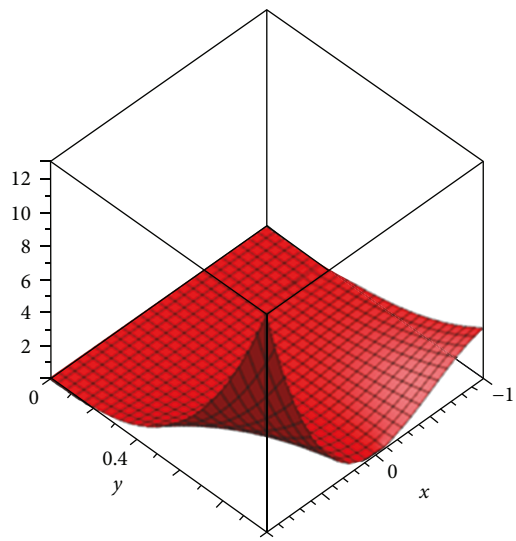

Figure 4: Plot of M-polynomial of NPHX[1,1].

Figure 4 shows the behavior of M-polynomial of NPHX[p, q], onto the involved parameters x, y.

Proposition 4. *For the H-naphtalenic nanotubes* NPHX[p, q], *we have*

$$\begin{aligned}
M_1(\mathrm{NPHX}[p,q]) &= 90pq + 20p,\\
M_2(\mathrm{NPHX}[p,q]) &= 135pq - 42p,\\
{}^{m}M_2(\mathrm{NPHX}[p,q]) &= \frac{5}{3}pq + \frac{2}{9}p,\\
R_\alpha(\mathrm{NPHX}[p,q]) &= 3^\alpha 3^\alpha 15pq - 10p3^{2\alpha} + 8p2^\alpha 3^\alpha,\\
R_\alpha(\mathrm{NPHX}[p,q]) &= \frac{1}{3^{2\alpha}}(15pq - 10p) + \frac{8}{2^\alpha \cdot 3^\alpha}p,\\
\mathrm{SSD}(\mathrm{NPHX}[p,q]) &= -\frac{8}{3}p + 30pq,\\
H(\mathrm{NPHX}[p,q]) &= -\frac{2}{5}p + 5pq,\\
I(\mathrm{NPHX}[p,q]) &= \frac{45}{2}pq - \frac{27}{5}p,\\
A(\mathrm{NPHX}[p,q]) &= \frac{10935}{64}pq - \frac{1597}{32}p.
\end{aligned} \tag{32}$$

Proof 4. Let

$$M(G;x,y) = f(x,y) = 8px^2y^3 + (15pq - 8p)x^2y^3. \tag{33}$$

Then,

$$\begin{aligned}
D_x f(x,y) &= 16px^2y^3 + 3(15pq - 10p)x^3y^3,\\
D_y f(x,y) &= 24px^2y^3 + 3(15pq - 10p)x^3y^3,\\
S_xS_y(f(x,y)) &= \frac{8}{6}px^2y^3 + \frac{1}{9}(15pq - 10p)x^3y^3,\\
D_x^aD_y^a(f(x,y)) &= 2^\alpha 3^\alpha 8px^2y^3 + 3^{2\alpha}(15pq - 10p)x^3y^3,\\
S_x^aS_y^a(f(x,y)) &= \frac{8}{2^\alpha 3^\alpha}px^2y^3 + \frac{1}{3^{2\alpha}}(15pq - 10p)x^3y^3,\\
S_yD_x(f(x,y)) &= \frac{16}{3}px^2y^3 + (15pq - 10p)x^3y^3,\\
2S_xJf(x,y) &= 2\left[\frac{8}{5}px^5 + \frac{1}{6}(15pq - 10p)x^6\right],\\
S_xJD_xD_yf(x,y) &= \frac{48}{5}px^5 + \frac{9}{6}(15pq - 10p)x^3y^3,\\
S_x^3Q_{-2}JD_x^3D_y^3f(x,y) &= \frac{1728}{27}px^3 - \frac{7290}{64}(15pq - 10p)x^4.
\end{aligned} \tag{34}$$

(1) First Zagreb index

$$\begin{aligned}
M_1(\mathrm{NPHX}[p,q]) &= (D_x + D_y)f(x,y)\big|_{x=y=1}\\
&= 6(15pq - 10p) + 24p
\end{aligned} \tag{35}$$

(2) Second Zagreb index

$$\begin{aligned}
M_2(\mathrm{NPHX}[p,q]) &= D_yD_x(f(x,y))\big|_{x=y=1}\\
&= 9(15pq - 10p) + 48p
\end{aligned} \tag{36}$$

(3) Modified second Zagreb index

$$\begin{aligned}
{}^{m}M_2(\mathrm{NPHX}[p,q]) &= S_xS_y(f(x,y))\big|_{x=y=1}\\
&= \frac{1}{9}p + \frac{1}{6}(15pq - 10p)
\end{aligned} \tag{37}$$

(4) Generalized Randić index

$$\begin{aligned}
R_\alpha(\mathrm{NPHX}[p,q]) &= D_x^\alpha D_y^\alpha(f(x,y))\Big|_{x=y=1}\\
&= 3^{2\alpha}(15pq - 10p) + 2^\alpha \cdot 3^\alpha(8p)
\end{aligned} \tag{38}$$

(5) Inverse Randić index

$$\begin{aligned}
RR_\alpha(\mathrm{NPHX}[p,q]) &= S_x^\alpha S_y^\alpha(f(x,y))\Big|_{x=y=1}\\
&= \frac{1}{3^{2\alpha}}(15pq - 10p) + \frac{1}{2^\alpha \cdot 3^\alpha}8p
\end{aligned} \tag{39}$$

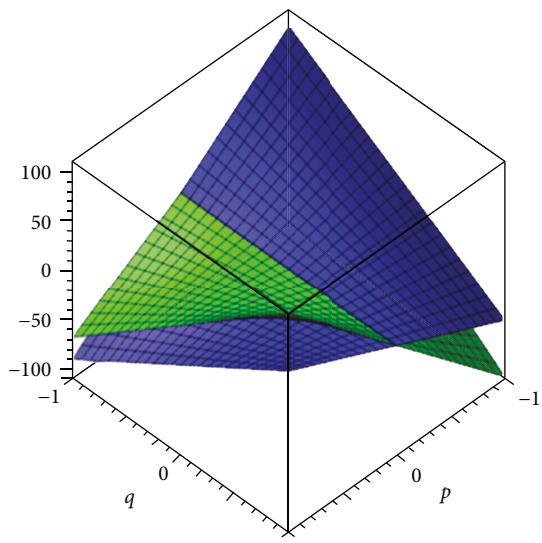

Figure 5: Plots of first Zagreb indices.

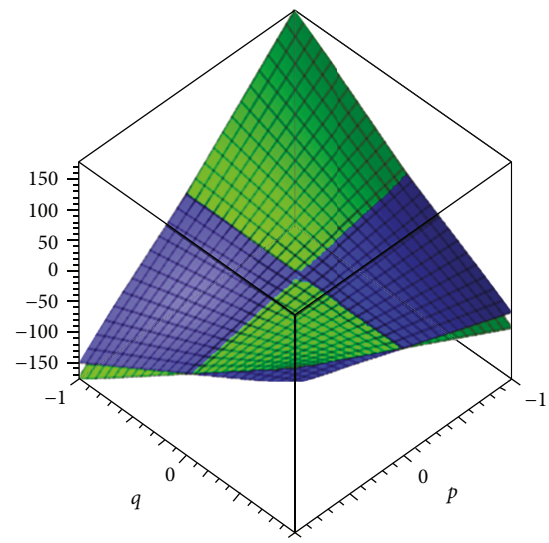

Figure 6: Plots of second Zagreb indices.

(6) Symmetric division index

$$\begin{aligned}\mathrm{SSD}(\mathrm{NPHX}[p,q]) &= \left(S_yD_x + S_xD_y\right)(f(x,y))\big|_{x=y=1}\\ &= 2(15pq) - \frac{8}{3}p\end{aligned} \tag{40}$$

(7) Harmonic index

$$H(\mathrm{NPHX}[p,q]) = 2S_xJ(f(x,y))|_{x=1} = \frac{1}{6}(15pq - 10p) + \frac{1}{5}8p \tag{41}$$

(8) Inverse sum index

$$\begin{aligned}I(\mathrm{NPHX}[p,q]) &= S_xJD_xD_y(f(x,y))_{x=1}\\ &= \frac{3}{2}(15pq - 10p) + \frac{48}{5}p\end{aligned} \tag{42}$$

(9) Augmented Zagreb index

$$\begin{aligned}A(\mathrm{NPHX}[p,q]) &= S_x^3Q_{-2}JD_x^3D_y^3(f(x,y))\Big|_{x=1}\\ &= \frac{10935}{64}pq - \frac{1597}{32}p\end{aligned} \tag{43}$$

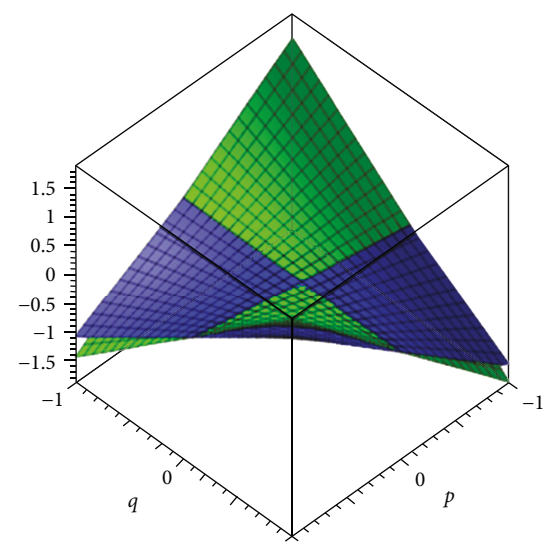

Figure 7: Plots of modified second Zagreb indices.

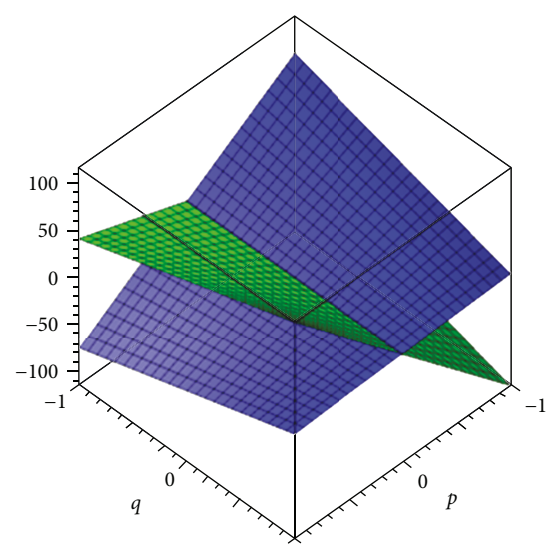

Figure 8: Plots of generalized Randić indices for alpha = 1/2.

4. Discussion and Concluding Remarks

We computed M-polynomials of $SC_5C_7[p,q]$ and $\mathrm{NPHX}[p,q]$. From these M-polynomials, we recovered nine degree-based topological indices by applying fundamental rules of calculus. Our calculated results help to understand topology of understudy nanotubes. For instant, the first Zagreb index is used to known about pi-electronic energy. Augmented Zagreb index can be used in the investigation of the heat of formation. Randić index is the most applied and investigated degree-based topological index. Figures 5–13 show the

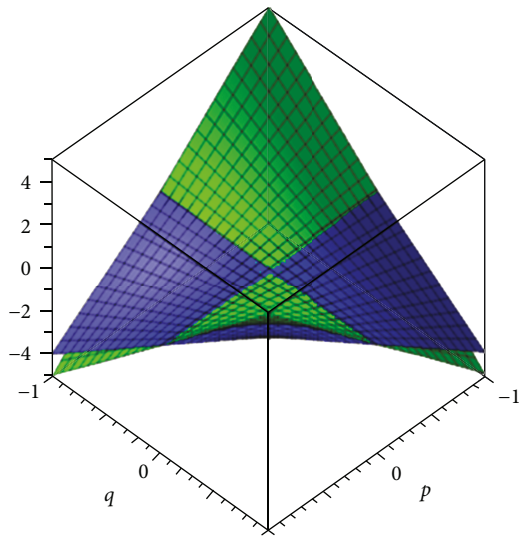

Figure 9: Plots of inverse Randić indices for alpha = 1/2.

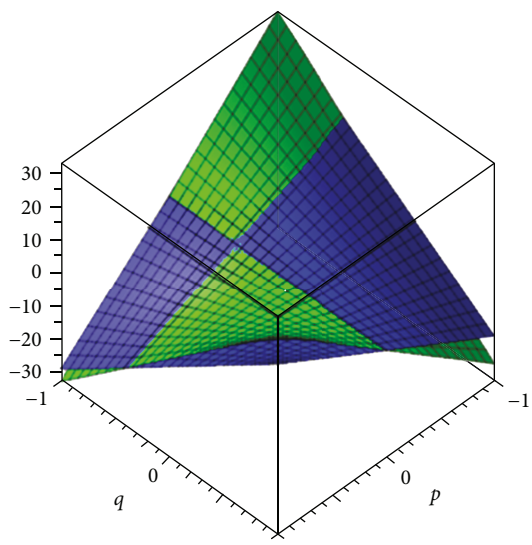

Figure 10: Plots of symmetric division indices.

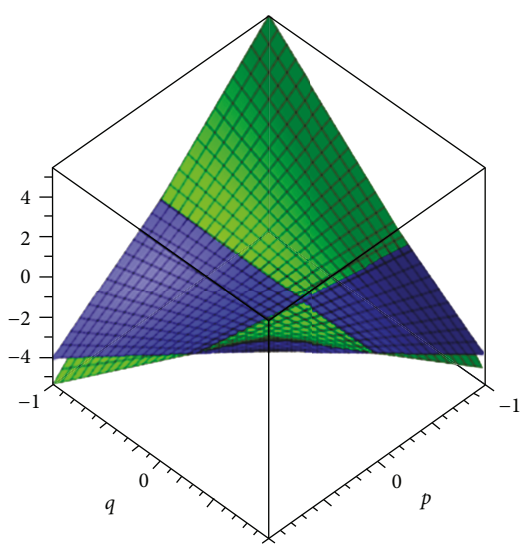

Figure 11: Plots of harmonic indices.

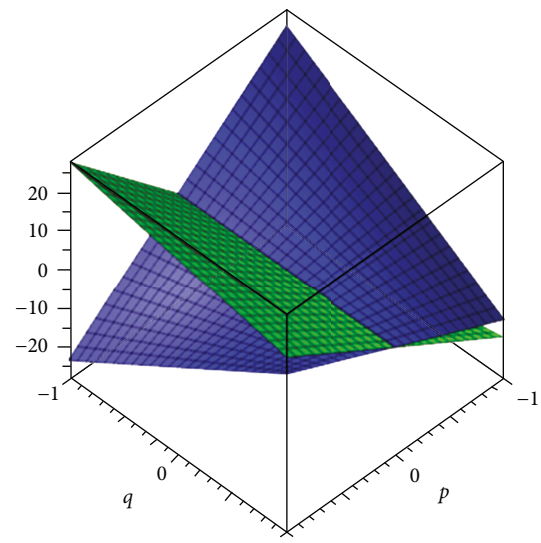

Figure 12: Plots of inverse sum indices.

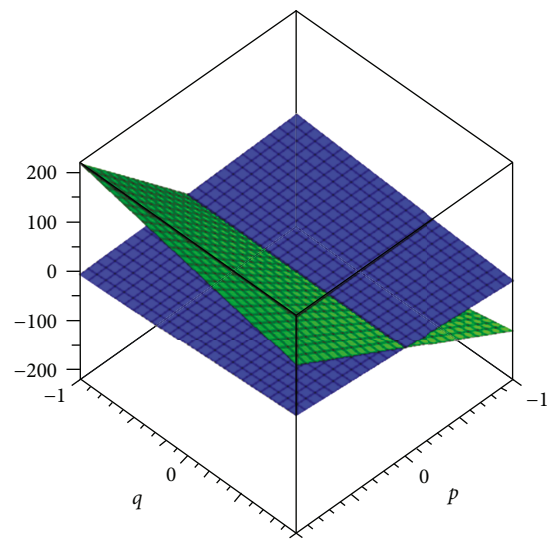

Figure 13: Plots of augmented Zagreb indices.

dependence of our results on the involved parameters. Blue color is fixed for $SC_5C_7[p, q]$, and green color is fixed for $NPHX[p, q]$.

Data Availability

All data is included within this paper.

Conflicts of Interest

The authors do not have any competing interests.

Authors' Contributions

All authors contribute equally in this paper.

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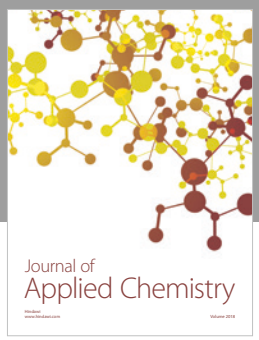

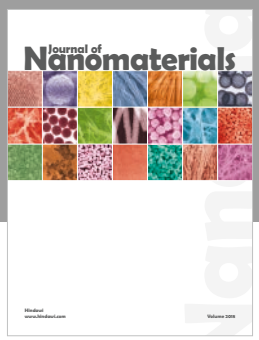

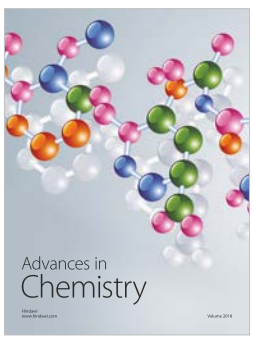

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