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Investigating new Revan indices on V-Phenylenic nanotube and nanotori with M-polynomial approach

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Abstract

V-Phenylenic nanotubes *VPNTU[l,k]* and nanotori *VPNTO[l,k]* are theoretically predicted carbon-based nanostructures with promising electronic and mechanical properties. While experimental synthesis remains elusive, computational studies suggest they could exhibit exceptional conductivity, strength, and potential applications in electronic and materials science.

In this article, the new Revan indices (*RI*) for molecular graph (*MG*), line graph (*LG*) and subdivision graph (*SG*) of *VPNTU [l, k]* and *VPNTO [l, k]* are investigated. By utilizing M-polynomial obtained from *MG*, *LG* and *SG* and MATLAB software coding, calculations and results obtained from research are presented.

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

Keywords: *Revan indices, M-polynomial, Nanotube, VPNTU [l, k], Line graph, Subdivision graph.*

1. Introduction

Carbon nanotubes(*CNT*), which were discovered in 1985, are one of the popular materials in the field of technology and are widely studied due to their properties, low implementation cost, and significant electron transfer [19].

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One of the fundamental characteristics of *CNTs* is their molecular structure, which has a diameter measured in nanometers and a large length-to-diameter ratio. Carbon nanotubes, initially discovered in 1985, have emerged as a prominent material in the realm of technology due to their exceptional properties, low production costs, and efficient electron transport. Their unique molecular structure, characterized by a nanometer-scale diameter and a substantial length-to-diameter ratio, coupled with increasing production capacity and decreasing prices, has fueled their widespread research and application [2, 8, 30, 31].

The safe switching capability properties of *CNTs* make them highly promising for the upgrade electronic devices on the nano scale, including transistors, multi-terminal nanoelectronics, amplifiers, and more. Their diverse applications extend beyond electronics, encompassing nanoelectric devices, lithium-ion batteries, membranes, electrochemical energy storage systems, chemical and biochemical sensors, and optoelectronic devices [6].

The exceptional mechanical, electrical, and catalytic properties of *CNTs*, attributed to their high specific surface area, have led to their widespread use in various fields. When incorporated into polymers to create composites, *CNTs* offer enhanced conductivity compared to carbon black composites, resulting in improved performance. Moreover, their geometric properties have demonstrated significant potential in drug delivery, electron field emission, battery electrodes, and voltage hysteresis applications [6].

Comprehensive research has been conducted on *VPNTU [l, k]* and *VPNTO [l, k]* nanostructures, revealing their suitability for catalysis, gas sensing, and corrosion resistance. Mathematical chemistry (*MC*) is a branch of mathematics in which chemical compounds are studied by relating them to diagrams. A topological index (*TI*) acts as a mathematical variable that elucidates the underlying topological arrangement of molecules or networks [28].

Figure (1) shows the *MG* of the *VPNTU[l,k].*

VPNTU [l, k] particles, characterized by l atoms in rows and k atoms in columns, have emerged as promising candidates for nanophotonics. We denote V-Phenylenic nanotube and nanotori as *VPNTU [l, k]* and *VPNTO [l, k]*, respectively. The molecular graph of *VPNTO [l, k]* is depicted in Figure 2.

Pi-polynomials and topological indices associated with *VPNTU[l, k]* and *VPNTO[l, k]* have been extensively studied [1, 12]. Several well-known *TIs*, including the *Pi* vertex index [3], geometric-arithmetic index and

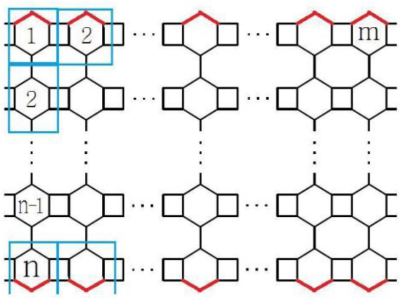

Figure 1

The *MG* of *VPNTU [l, k]*.

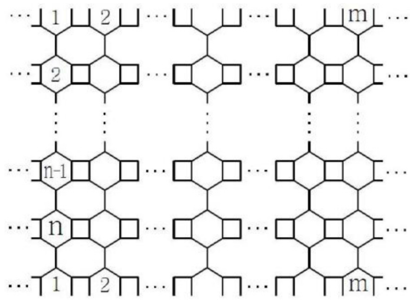

Figure 2

The *MG* of *VPNTO [l, k]*.

atom-bond connectivity index [16], eccentricity connectivity index [32], Zagreb indices [9, 10], M-polynomials [28], and Laplacian and signless Laplacian spectra [21], have been calculated for these nanostructures.

MC, a subfield of theoretical chemistry, employs mathematical methods to analyze molecular structure without delving into quantum mechanics.

TI play a pivotal role in this discipline. Chemical graph theory is a mathematical approach in chemistry that uses graph theory to model molecules, representing atoms as vertices and bonds as edges in a molecular graph.

In the fields of *MC*, the *TI* is a numerical quantity obtained from the connection patterns of graphs and has found wide applications, especially in medicine and pharmaceuticals. Recent research has extensively explored the application of *TI* in chemical studies [11, 12, 14, 22, 29, 34].

In this article, we employ M-polynomials to calculate the product connectivity Revan, forgotten Revan (*F*-Revan), symmetric division Revan, harmonic Revan, and inverse sum indeg Revan indices. Subsequently, the Revan indices for the molecular graphs of *VPNTU [l, k]* and *VPNTO [l, k]* are computed and the corresponding M-polynomials are plotted. Finally, a comparative analysis of these numerical quantities is conducted, with the product connectivity Revan index being derived from M-polynomials using MATLAB coding.

2. Preliminaries

This section provides some of the required definitions.

Definition 2.1: In a non-empty graph *N*, the line graph *L(N)* is constructed by considering each edge of *N* as a vertex [7].

Definition 2.2: The subdivision graph *S(N)* of a graph *N* is constructed by subdividing each edge of *N* with a single vertex [7].

Numerous graph polynomials have been introduced to date [13, 17, 37], many of which have proven valuable in the field of mathematical chemistry. These graph polynomials have yielded significant insights into chemical networks and their associated topological indices. Researchers have leveraged these results to establish meaningful correlations between chemical compounds and their corresponding chemical and biological properties. Among the most commonly employed graph polynomials, the M-polynomial stands out as a prominent tool.

Definition 2.3: Suppose *N* be a graph, and let $\mathrm{M}_{f,z}$, $f,z \geq 1$ be the number of edges *lk* of *N* such that $\{d_l, d_k\} = \{f, z\}$. The M-polynomial of *N* is obtained as follows [5]:

$$M(N,r,s) = \sum_{\delta \leq f \leq z \leq \Delta} \mathrm{M}_{f,z} r^f s^z.$$

The following operators are used in the subsequent theorems.

$$D_r = r \times \frac{\partial M\ (N,r,s)}{\partial r},\ D_s = s \times \frac{\partial M\ (N,r,s)}{\partial s},\ Q_{\mathrm{r}(a)} M\ (N,r,s) = r^a.M\ (N,r,s),$$

$$Q_{s(a)} M\ (N,r,s) = s^a.M\ (N,r,s),\ S_r M\ (N,r,s) = \int_0^r \frac{M(N,t,s)}{t} dt,$$

$$S_s M\ (N,r,s) = \int_0^s \frac{M(N,r,t)}{t} dt,\ JM(N,r,s) = M(N,r,r).$$

The M-polynomial provides a powerful tool for computing *TIs*. By employing mathematical manipulations such as derivatives and integrals with respect to the variables x and y, various *TIs* can be derived from the M-polynomial. The application of this approach to molecular graphs has been the subject of numerous investigations [4, 18, 20, 33].

Definition 2.4: The first and second Revan index (*RI)* of a graph *N* were introduced as follows [21]:

$$R_1(N) = \sum_{lk \in E(N)} [r_l + r_k],\quad R_2(\mathrm{N}) = \sum_{lk \in E(\mathrm{N})} [r_l . r_k].$$

where the degree of Revan for vertex *l* in graph *N* is expressed as $r_l = \Delta + \delta - \mathrm{d}_l$ and Δ represents the maximum and δ the minimum degrees of the vertex of N, respectively. Extensive research has been conducted on the Randić index [15, 26, 27].

Definition 2.5: The product connectivity *RI* was introduced as follows [23]:

$$PR(G) = \sum_{lk \in E(G)} \frac{1}{\sqrt{r_l \cdot r_k}}.$$

Definition 2.6: The forgotten Revan (F-Revan) index can be expressed as follows in [24]:

$$FR(G) = \sum_{lk \in E(G)} [r_l^2 + r_k^2].$$

Definition 2.7: The symmetric division *RI* can be expressed as follows in [24]:

$$SDR(G) = \sum_{lk \in E(G)} \left[\frac{r_l}{r_k} + \frac{r_k}{r_l}\right].$$

Definition 2.8: The harmonic *RI* can be expressed as follows in [25]:

$$HR(G) = \sum_{lk \in E(G)} \frac{2}{r_l + r_k}.$$

Definition 2.9: The inverse sum indeg *RI* can be expressed as follows in [25]:

$$IR(G) = \sum_{lk \in E(G)} \frac{r_l . r_k}{r_l + r_k}.$$

3. Relationship between M-polynomial and some *RI*

Theorem 3.1: *Suppose $M(N, r, s)$ denote the M-polynomial the graph N. Then the product connectivity RI is computed as,*

$$PR(N) = [D_r^{-\frac{1}{2}} D_s^{-\frac{1}{2}} (Q_{r(-\Delta-\delta)} Q_{s(-\Delta-\delta)} M\ (N, r, s))\big|_{(r,s)=(1,1)}].$$

Proof:

$$PR(N) = \sum_{lk \in E(N)} \frac{1}{\sqrt{r_l . r_k}} = \sum_{lk \in E(G)} \frac{1}{\sqrt{(\Delta+\delta-d_l).(\Delta+\delta-d_k)}} = \sum_{lk \in E(G)} \frac{1}{\sqrt{(d_l-\Delta-\delta).(d_k-\Delta-\delta)}}, \qquad (2)$$

$$Q_{r(-\Delta-\delta)}Q_{s(-\Delta-\delta)}M(N,r,s)=\sum_{\delta\le i\le j\le\Delta}M_{ij}r^{(i-\Delta-\delta)}s^{(j-\Delta-\delta)},$$

$$D_s^{-\frac{1}{2}}(\sum_{\delta\le i\le j\le\Delta}M_{ij}r^{i-\Delta-\delta}s^{j-\Delta-\delta})=\sum_{\delta\le i\le j\le\Delta}M_{ij}r^{(i-\Delta-\delta)}\frac{1}{\sqrt{(j-\Delta-\delta)}}(s^{(j-\Delta-\delta)})^{-\frac{1}{2}},$$

$$D_r^{-\frac{1}{2}}D_s^{-\frac{1}{2}}(\sum M_{i,j}r^{(i-\Delta-\delta)}s^{(j-\Delta-\delta)})=\sum_{\delta\le i\le j\le\Delta}M_{ij}\frac{1}{\sqrt{(i-\Delta-\delta)(j-\Delta-\delta)}}(r^{(i-\Delta-\delta)})^{-\frac{1}{2}}.(s^{(j-\Delta-\delta)})^{-\frac{1}{2}}$$

$$D_r^{-\frac{1}{2}}D_s^{-\frac{1}{2}}(\sum M_{i,j}r^{(i-\Delta-\delta)}s^{(j-\Delta-\delta)})\Big|_{(r,s)=(1,1)}=\sum_{\delta\le i\le j\le\Delta}M_{i,j}\frac{1}{\sqrt{(i-\Delta-\delta)(j-\Delta-\delta)}},\tag{3}$$

Hence, according to relations (2) and (3), we have

$$PR(N)=[D_r^{-\frac{1}{2}}D_s^{-\frac{1}{2}}(Q_{r(-\Delta-\delta)}Q_{s(-\Delta-\delta)}M\ (N,r,s))]\Big|_{(r,s)=(1,1)}.$$

Theorem 3.2: *Suppose* $M(N,r,s)$ *denote the M-polynomial the graph N. Then the F-Revan index is computed as,*

$$FR(N)=(D_r^2+D_s^2)(Q_{r(-\Delta-\delta)}Q_{s(-\Delta-\delta)}M\ (N,r,s))\Big|_{(r,s)=(1,1)}.$$

Proof:

$$FR(N)=\sum_{lk\in E(N)}(\Delta+\delta-d_l)^2+(\Delta+\delta-d_k)^2]=$$
$$\sum_{lk\in E(N)}(d_l-\Delta-\delta)^2+(d_k-\Delta-\delta)^2],\tag{4}$$

$$Q_{r(-\Delta-\delta)}Q_{s(-\Delta-\delta)}M\ (N,r,s)=\sum_{\delta\le i\le j\le\Delta}M_{i,j}r^{(i-\Delta-\delta)}s^{(j-\Delta-\delta)},$$

$$D_r^2(\sum M_{i,j}r^{(i-\Delta-\delta)}s^{(j-\Delta-\delta)})+D_s^2(\sum_{\delta\le i\le j\le\Delta}M_{i,j}r^{(i-\Delta-\delta)}s^{(j-\Delta-\delta)})=$$
$$\sum_{\delta\le i\le j\le\Delta}M_{i,j}.[(i-\Delta-\delta)^2+(j-\Delta-\delta)^2]r^{(i-\Delta-\delta)}\ .\ s^{(j-\Delta-\delta)},$$

$$D_r^2(\sum_{\delta\le i\le j\le\Delta}M_{i,j}r^{(i-\Delta-\delta)}s^{(j-\Delta-\delta)})+D_s^2(\sum_{\delta\le i\le j\le\Delta}M_{i,j}r^{(i-\Delta-\delta)}s^{(j-\Delta-\delta)})\Big|_{(r,s)=(1,1)}$$
$$=\sum_{\delta\le i\le j\le\Delta}M_{i,j}.[(i-\Delta-\delta)^2+(j-\Delta-\delta)^2],\tag{5}$$

Hence, according to relations (4) and (5), we have

$$FR(N) = [(D_r^2 + D_s^2)(Q_{r(-\Delta-\delta)}Q_{s(-\Delta-\delta)}M \ \ (N,r,s))]\Big|_{(r,s)=(1,1)}.$$

Theorem 3.3: *Suppose* $M(N,r,s)$ *denote the M-polynomial the graph N. Then the symmetric division RI is computed as,*

$$SDR(N) = (D_r S_s + S_r D_s)(Q_{r(-\Delta-\delta)}Q_{s(-\Delta-\delta)} \ M \ \ (N,r,s))\Big|_{(r,s)=(1,1)}.$$

Proof:

$$SDR(N) = \sum_{lk\in E(N)} \frac{d_l-\Delta-\delta}{d_k-\Delta-\delta} + \frac{d_k-\Delta-\delta}{d_l-\Delta-\delta}\Big), \tag{6}$$

$$D_s(\sum_{\delta\le i\le j\le\Delta} M_{i,j} r^{(i-\Delta-\delta)} s^{(j-\Delta-\delta)}) = \sum_{\delta\le i\le j\le\Delta} M_{i,j}(j-\Delta-\delta) r^{(i-\Delta-\delta)} s^{(i-\Delta-\delta)},$$

$$\begin{aligned} S_r D_s(\sum_{\partial\le i\le j\le\Delta} M_{i,j} r^{(i-\Delta-\delta)} s^{(j-\Delta-\delta)}) &= \sum_{\partial\le i\le j\le\Delta} (M_{i,j}(j-\Delta-\delta) s^{(j-\Delta-\delta)} \int_0^r \frac{t^{(i-\Delta-\delta)}}{t} dt), \\ &= \sum_{\partial\le i\le j\le\Delta} M_{i,j}(j-\Delta-\delta) s^{(j-\Delta-\delta)} \frac{r^{(i-\Delta-\delta)}}{(i-\Delta-\delta)}, \\ &= \sum_{\partial\le i\le j\le\Delta} M_{i,j} \frac{(j-\Delta-\delta)}{(i-\Delta-\delta)} r^{(i-\Delta-\delta)} . s^{(j-\Delta-\delta)}, \end{aligned}$$

$$\begin{aligned} S_r D_s(\sum_{\partial\le i\le j\le\Delta} M_{i,j} r^{(i-\Delta-\delta)} s^{(j-\Delta-\delta)}) &= \sum_{\partial\le i\le j\le\Delta} (M_{i,j}(i-\Delta-\delta) r^{(j-\Delta-\delta)} \int_0^s \frac{t^{(j-\Delta-\delta)}}{t} dt), \\ &= \sum_{\partial\le i\le j\le\Delta} M_{i,j}(i-\Delta-\delta) r^{(i-\Delta-\delta)} \frac{s^{(j-\Delta-\delta)}}{(j-\Delta-\partial)}, \\ &= \sum_{\partial\le i\le j\le\Delta} M_{i,j} \frac{(i-\Delta-\delta)}{(j-\Delta-\delta)} r^{(i-\Delta-\delta)} . s^{(j-\Delta-\delta)}, \end{aligned}$$

$$(S_r D_s + S_s D_r)(\sum_{\delta\le i\le j\le\Delta} M_{i,j} r^{(i-\Delta-\delta)} s^{(j-\Delta-\delta)})\Big|_{(r,s)=(1,1)} = \sum_{\delta\le i\le j\le\Delta} M_{i,j}\left(\frac{(i-\Delta-\delta)}{(j-\Delta-\delta)} + \frac{(j-\Delta-\delta)}{(i-\Delta-\delta)}\right), \tag{7}$$

Hence, according to relations (6) and (7), we have

$$SDR(N) = (S_r D_s + S_s D_r)(\sum_{\delta\le i\le j\le\Delta} M_{i,j} r^{(i-\Delta-\delta)} s^{(j-\Delta-\delta)})\Big|_{(r,s)=(1,1)}.$$

Theorem 3.4: *Suppose M(N,r,s) denote the M-polynomial associated with the graph N. Then the harmonic RI is computed as,*

$$HR(N) = (-2S_r.J.Q_{r(-\Delta-\delta)}Q_{s(-\Delta-\delta)}\, M\ \ (N,r,s))\Big|_{r=1}.$$

Proof:

$$HR(N) = \sum_{lk\in E(N)} \frac{2}{r_l+r_k} = 2\sum_{lk\in E(N)} \frac{1}{r_l+r_k} = -2\sum_{\delta\le i\le j\le\Delta} \frac{1}{(d_l-\Delta-\delta)+(d_k-\Delta-\delta)}, \tag{8}$$

$$J(\sum_{\delta\le i\le j\le\Delta} M_{i,j} r^{(i-\Delta-\delta)} s^{(j-\Delta-\delta)}) = \sum_{\delta\le i\le j\le\Delta} M_{i,j} r^{(i-\Delta-\delta)} s^{(j-\Delta-\delta)},$$

$$S_r.J(\sum_{\delta\le i\le j\le\Delta} M_{i,j} r^{(i-\Delta-\delta)} s^{(j-\Delta-\delta)}) = \sum_{\delta\le i\le j\le\Delta} M_{i,j}\int_0^r \frac{t^{(i+j-2\Delta-2\delta)}}{t}dt,$$

$$= (-2S_r J(\sum_{\delta\le i\le j\le\Delta} M_{i,j} r^{(i-\Delta-\delta)} s^{(j-\Delta-\delta)}\ )\Big|_{(r=1)},$$

$$= -2\sum_{\delta\le i\le j\le\Delta} M_{i,j}\frac{1}{(i-\Delta-\delta)+(j-\Delta-\delta)}, \tag{9}$$

Hence, according to relations (8) and (9), we have

$$HR(N) = (-2S_r.J.Q_{r(-\Delta-\delta)}Q_{s(-\Delta-\delta)}\, M\ \ (N,r,s))\Big|_{r=1}.$$

Theorem 3.5: *Suppose M(N,r,s) denote the M-polynomial associated with the graph N. Then the inverse sum indeg RI is computed as,*

$$IR(N) = -(S_r J D_r D_s)Q_{r(-\Delta-\delta)}Q_{s(-\Delta-\delta)}\, M\ \ (N,r,s))\Big|_{r=1}.$$

Proof:

$$IR(N) = \sum_{lk\in E(N)} \frac{r_l.r_k}{r_l+r_k} = -\sum_{lk\in E(N)} \frac{(d_l-\Delta-\delta).(d_k-\Delta-\delta)}{(d_l-\Delta-\delta)+(d_k-\Delta-\delta)}, \tag{10}$$

$$D_r.D_s(\sum_{\delta\le i\le j\le\Delta} M_{i,j} r^{(i-\Delta-\delta)} s^{(j-\Delta-\delta)}) = \sum_{\delta\le i\le j\le\Delta} M_{i,j}(i-\Delta-\delta)(j-\Delta-\delta) r^{(i-\Delta-\delta)} s^{(j-\Delta-\delta)},$$

$$JD_rD_s(\sum_{\delta\le i\le j\le\Delta} M_{i,j} r^{(i-\Delta-\delta)} s^{(j-\Delta-\delta)}) = \sum_{\delta\le i\le j\le\Delta} M_{i,j}(i-\Delta-\delta)(j-\Delta-\delta) r^{(i-\Delta-\delta)} r^{(j-\Delta-\delta)},$$

$$-S_r JD_rD_s(\sum_{\delta\le i\le j\le\Delta} M_{i,j} r^{(i-\Delta-\delta)} s^{(j-\Delta-\delta)}\ \ )\Big|_{r=1}$$

$$= \left[-\sum_{\delta\le i\le j\le\Delta} M_{i,j}(i-\Delta-\delta)(j-\Delta-\delta)\int_0^r \frac{t^{i+j-2\Delta-2\delta}}{t}dt\Big|\right]_{r=1},$$

$$= -\sum_{\delta \le i \le j \le \Delta} M_{i,j} \frac{(i-\Delta-\delta)(j-\Delta-\delta)}{(i+j-2\Delta-2\delta)}, \tag{11}$$

Hence, according to relations (10) and (11), we have

$$IR(N) = -(S_r J D_r D_s) Q_{r(-\Delta-\delta)} Q_{s(-\Delta-\delta)} M\ (N, r, s))\Big|_{r=1}.$$

Based on the aforementioned theorems, Table (1) was constructed to compute the *RI* utilizing the *M-PO* method.

Table 1
Derivation of *RI* from M-polynomial.

***TI* name**	**Derivation from *M(N, r, s)***
Product connectivity *RI*	$[D_r^{-\frac{1}{2}} D_s^{-\frac{1}{2}} (Q_{r(-\Delta-\delta)} Q_{s(-\Delta-\delta)} M\ (N, \mathrm{r}, s))]\Big|_{(r,s)=(1,1)}$
F-RI	$[(D_r^{2} + D_s^{2})(Q_{r(-\Delta-\delta)} Q_{s(-\Delta-\delta)} M\ (N, \mathrm{r}, s))]\Big|_{(r,s)=(1,1)}$
Symmetric division *RI*	$[(D_r S_s + S_r D_s)(Q_{r(-\Delta-\delta)} Q_{s(-\Delta-\delta)} M\ (N, r, s))]\Big|_{(r,s)=(1,1)}$
Harmonic *RI*	$[(-2S_r . J . Q_{r(-\Delta-\delta)} Q_{s(-\Delta-\delta)} M\ (N, r, s))]\Big|_{r=1}$
Inverse sum *RI*	$[-(S_r J D_r D_s) Q_{r(-\Delta-\delta)} Q_{r(-\Delta-\delta)} M\ (N, r, s))]\Big|_{r=1}$

4. *VPNTU [l, k]* and *VPNTO [l, k]*

In this article, *MG* of *VPNTU [l, k]* and *VPNTO [l, k]* are shown with *G* and *H*, respectively.

There are two edge partitions $E_1 = \{lk \in E(G) \mid d_l = 2,\ d_k = 3\}$ and $E_2 = \{lk \in E(G) \mid\mid d_k = 3,\ d_l = 3\}$ in *MG* of the *VPNTU* with the number of $|E_1| = 4l$ and $|E_2| = 9lk - 5l$.

Figure (3) shows the *LG* of the *VPNTU.*

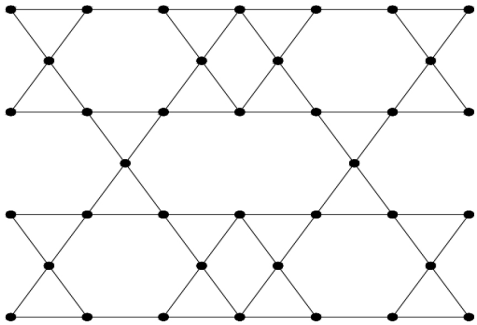

Figure 3

L(G) **in** *VPNTU [2, 2].*

There are three edge partitions $E_1' = \{lk \in E(L(G)) \mid d_l = 3,\ d_k = 3\}$ $E_2' = \{lk \in E(L(G)) \mid d_l = 3,\ d_k = 4\}$ and $E_3' = \{lk \in E(L(G)) \mid d_l = 4,\ d_k = 4\}$ in *LG* of the *VPNTU* with the number of $|E_1'| = 2l$, $|E_2'| = 8l$ and $|E_3'| = 18lk - 14l$.

Consequently, the quantity of edges and vertices within the [full definition of *LG* of the *VPNTU [l, k]*] is:

$$\left|E(L(G))\right| = 18lk - 4l.$$

$$\left|V(L(G))\right| = \left|E(G)\right| = 9lk - l.$$

Figure (4) shows the *SG* of the *VPNTU [l, k]*.

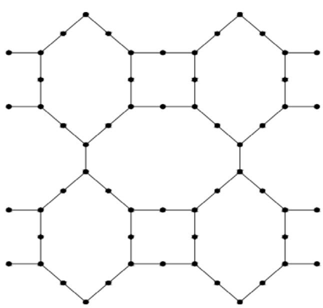

Figure 4

***S(G)* in *VPNTU* [2, 2].**

There are two edge partitions $E_1'' = \{lk \in E(S(G)) \mid d_l = 2,\ d_k = 2\}$ $E_2'' = \{lk \in E(S(G)) \mid d_l = 2,\ d_k = 3\}$ and $E_3' = \{lk \in E(S(G)) \mid d_l = 4,\ d_k = 4\}$ in *SG* of the *VPNTU* with the number of $|E_1'| = 2l$, $|E_2'| = 8l$ and $|E_3'| = 18lk - 6l$.

Consequently, the quantity of edges and vertices within the [full definition of *SG* of the *VPNTU [l, k]*] is:

$$|E(S(G))| = |E_1''| + |E_2''| = 4l + 18lk - 6l = 18lk - 2l,$$
$$|V(S(G))| = |E(G)| + |V(G)| = 15lk - l.$$

There are one edge partitions $\overline{E}_1 = \{lk \in E(H) \mid d_l = 3, d_k = 3\}$ in *MG* of the *VPNTO* with the number of $|\overline{E}_1| = 9lk$.

Figure (5) shows the *LG* of the *VPNTO.*

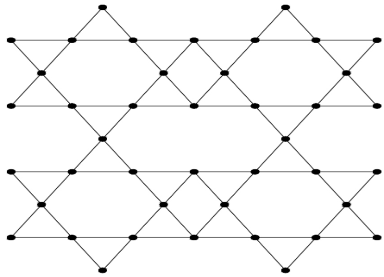

Figure 5

LG* of *VPNTO [2, 2].

There are one edge partitions $\overline{E}_1 = \{lk \in E(L(H)) \mid d_l = 3, d_k = 3\}$ in *LG* of the *VPNTO* with the number of $|\overline{E}_1| = 9l$.

As a result, we have:

$$|E(L(H))| = 18lk,$$
$$|V(L(H))| = |E(H)| = 9lk.$$

Figure (6) shows the *SG* of the *VPNTO.*

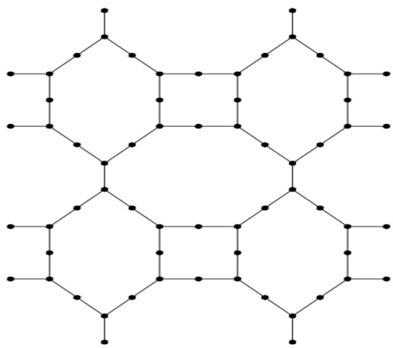

Figure 6

S(G)* in *VPNTO [2, 2].

There are one edge partitions $\overline{E}_1'' = \{lk \in E(S(H)) \mid d_l = 2, d_k = 3\}$ in *SG* of the *VPNTO* with the number of $|\overline{E}_1''| = 18lk$.

Consequently, the quantity of edges and vertices within the [full definition of *SG* of the *VPNTO [l, k]*] is:

$$|E(S(H))| = 18lk,$$
$$|V(S(H))| = |E(H)| + |V(H)| = 15lk.$$

5. Main Results

Theorem 5.1: *Suppose G, L(G) and S(G) denotes M-polynomial associated with the MG, LG and SG of the VPNTU [l, k]. Then M-polynomial are calculated as follows,*

$$M(G,x,y) = (4l)x^2y^3 + (9lk-5l)x^3y^3,$$
$$M(L(G),x,y) = (2l)x^3y^3 + (8l)x^3y^4 + (18lk-14l)x^4y^4,$$
$$M(S(G),x,y) = (4l)x^2y^2 + (18lk-6l)x^2y^3.$$

Proof: It is easily obtained by the definition 2.3 and the structure of *MG*, *LG* and *SG* of *VPNTU [l, k]*.

Theorem 5.2: *Suppose G denote the graph of the VPNTU [l, k]. Then new RI are calculated as follows,*

1. $PR(G) = \frac{9lk}{2} + \left(\frac{2\sqrt{6}}{3} - \frac{5}{2}\right)l,$
2. $FR(G) = 72lk + 12l,$
3. $SDR(G) = 18lk - \left(\frac{4}{3}\right)l,$
4. $HR(G) = \left(\frac{9}{2}\right)lk - \left(\frac{9}{10}\right)l,$
5. $IR(G) = 9lk - \left(\frac{1}{5}\right)l.$

Proof: By applying the operators of Table (1) to Theorem (5.1) we have:

$$Q_{x(-5)}Q_{y(-5)}M(G,x,y) = (4l)x^{-3}y^{-2} + (9lk-5l)x^{-2}y^{-2},$$

$$D_x^{-\frac{1}{2}}D_y^{-\frac{1}{2}}(Q_{x(-5)}Q_{y(-5)}M(H_1(n),x,y)) = \left(4l \times \frac{1}{\sqrt{6}}\right)x^{-3}\ .y^{-2} + \left((9lk-5l) \times \frac{1}{\sqrt{4}}\right)x^{-2}.y^{-2}$$

$$D_y^2Q_{x(-5)}Q_{y(-5)}M(G,x,y) = 2l.(-2)^2x^{-3}y^{-2} + (9lk-5l)\cdot(-2)^2x^{-2}y^{-2},$$

$$D_x^2 Q_{x(-5)} Q_{y(-5)} M(G,x,y) = 4l.(-3)^2 x^{-3} y^{-2} + (9lk-5l)\cdot(-2)^2 x^{-2} y^{-2},$$

$$D_x Q_{x(-5)} Q_{y(-5)} M(G,x,y) = 4l.(-3) x^{-3} y^{-2}\ ?+ (9lk-5l)\cdot(-2) x^{-2} y^{-2},$$
$$D_y Q_{x(-5)} Q_{y(-5)} M(G,x,y) = 4l.(-2) x^{-3} y^{-2} + (9lk-5l)\cdot(-2) x^{-2} y^{-2},$$

$$S_y (Q_{x(-5)} Q_{y(-5)} M\ (G,x,y)) = \int_0^y \frac{4lx^{-3}t^{-2}}{t} dt + \int_0^y \frac{(9lk-5l)x^{-2}t^{-2}}{t} dt = \frac{4l}{-2} x^{-3} y^{-2} + \frac{(9lk-5l)}{-2} x^{-2} y^{-2},$$

$$S_x D_y (Q_{x(-5)} Q_{y(-5)} M\ (G,x,y)) = \int_0^x \frac{(-8l)t^{-3}y^{-2}}{t} dt + \int_0^x \frac{(-2(9lk-5l))t^{-2}y^{-2}}{t} dt = \frac{8l}{3} x^{-3} y^{-2} + (9lk-5l) x^{-2} y^{-2},$$

$$J(Q_{x(-5)} Q_{y(-5)} M\ (G,x,y))) = 4lx^{-5} + (9lk-5l)x^{-4},$$
$$S_x J(Q_{x(-5)} Q_{y(-5)} M\ (G,x,y))) = \int_0^x \frac{4lt^{-5}}{t} dt + \int_0^x dt = \frac{-4l}{5} x^{-5} - \frac{(9lk-5l)x^{-4}}{4},$$
$$D_x D_y (Q_{x(-5)} Q_{y(-5)} M\ (G,x,y)) = 24lx^{-3} y^{-2} + 4(9lk-5l) x^{-2} y^{-2},$$

$$J D_x D_y (Q_{x(-5)} Q_{y(-5)} M\ (G,x,y)) = 24l(x^{-5}) + 4(9lk-5l)x^{-4},$$

$$S_x J D_x D_y (Q_{x(-5)} Q_{y(-5)} M\ (G,x,y)) = \int_0^x \frac{24lt^{-5}}{t} dt - \int_0^x \frac{4(9lk-5l)t^{-4}}{t} dt = \frac{-24l}{5} x^{-5} - (9lk-5l)x^{-4}.$$

1. $[D_x^{-\frac{1}{2}} D_y^{-\frac{1}{2}} (Q_{x(-5)} Q_{y(-5)} M(G,x,y))]\Big|(x,y) = (1,1) = \frac{9lk}{2} + \left(\frac{2\sqrt{6}}{3} - \frac{5}{2}\right) l,$
2. $[(D_x^2 + D_y^2)(Q_{x(-5)} Q_{y(-5)} M\ (G,x,y))]\Big|(x,y) = (1,1) = 72lk + 12l,$
3. $[(D_x S_y + S_x D_y)(Q_{x(-5)} Q_{y(-5)} M\ (G,x,y))]\Big|(x,y) = (1,1) = 18lk + \left(\frac{4}{3}\right) l,$
4. $[-2 S_x J(Q_{x(-5)} Q_{y(-5)} M\ (G,x,y))]\Big| x = 1 = \left(\frac{9}{2}\right) lk - \left(\frac{9}{10}\right) l,$
5. $[-S_x J D_x D_y (Q_{x(-5)} Q_{y(-5)} M\ (G,x,y))]\Big|\ x = 1 = 9lk - \left(\frac{1}{5}\right) l.$

Theorem 5.3: *Suppose L(G) denote the LG of the VPNTU [l, k]. Then new RI are calculated as follows,*

1. $PR(L(G)) = 9lk + \left(\frac{4\sqrt{3}-14}{3} + \frac{1}{2}\right) l,$
2. $FR(L(G)) = 324lk + 12l,$
3. $SDR(L(G)) = 36lk - \frac{22}{3} l,$

4. $HR(L(G)) = 6lk + \left(\frac{1}{2} + \frac{16}{7} - \frac{14}{3}\right)l,$
5. $IR(L(G)) = 27lk + \left(\frac{96}{7} - 17\right)l.$

Proof: It is easily obtained similar to Theorem 5.2.

Theorem 5.4: *Suppose S(G) denote the SG of the VPNTU [l, k]. Then new RI are calculated as follows,*

1. $PR(S(G)) = \frac{\sqrt{6}}{3} lk + \left(\frac{4}{3} - \sqrt{6}\right)l,$
2. $FR(S(G)) = 234lk - 6l,$
3. $SDR(S(G)) = 39lk - 2l,$
4. $HR(S(G)) = \frac{36}{5} lk - \frac{16}{15} l,$
5. $IR(S(G)) = \frac{108}{5} lk - \frac{6}{5} l.$

Proof: It is easily obtained similar to Theorem 5.2.

Theorem 5.5: *Suppose H, L(G) and S(G) denotes M-polynomial associated with the MG, LG and SG of the VPNTO [l, k]. Then M-polynomial are calculated as follows,*

$$M(H, x, y) = (9lk)x^4y^4,$$
$$M(L(H), x, y) = (18lk)x^4y^4,$$
$$M(S(H), x, y) = (18k)x^2y^3.$$

Proof: It is easily obtained by the definition 2.3 and the structure of MG, LG and *SG* of *VPNTO [l, k].*

Theorem 5.6: *Suppose H denote the graph of the VPNTO [l, k]. Then new RI are calculated as follows,*

1. $PR(H) = lk,$
2. $FR(H) = 162lk,$
3. $SDR(H) = 18lk,$
4. $HR(H) = 3lk,$
5. $IR(H) = \frac{27}{2} lk.$

Proof: It is easily obtained similar to Theorem 5.2.

Theorem 5.7: *Suppose L(H) denote the LG of the VPNTO [l, k]. Then new RI are calculated as follows,*

1. $PR(L(H)) = \frac{9}{2}lk$,
2. $FR(L(H)) = 576lk$,
3. $SDR(L(H)) = 36lk$,
4. $HR(L(H)) = \left(\frac{9}{2}\right)lk$,
5. $IR(L(H)) = 36lk$.

Proof: It is easily obtained similar to Theorem 5.2. □

Theorem 5.8: *Suppose S(H) denote the SG of the VPNTO [l, k]. Then new RI are calculated as follows,*

1. $PR(S(H)) = 3\sqrt{6}lk$,
2. $FR(S(H)) = 234lk$,
3. $SDR(S(H)) = 39lk$,
4. $HR(S(H)) = \left(\frac{36}{5}\right)lk$,
5. $IR(S(H)) = \left(\frac{108}{5}\right)lk$.

Proof: It is easily obtained similar to Theorem 5.2.

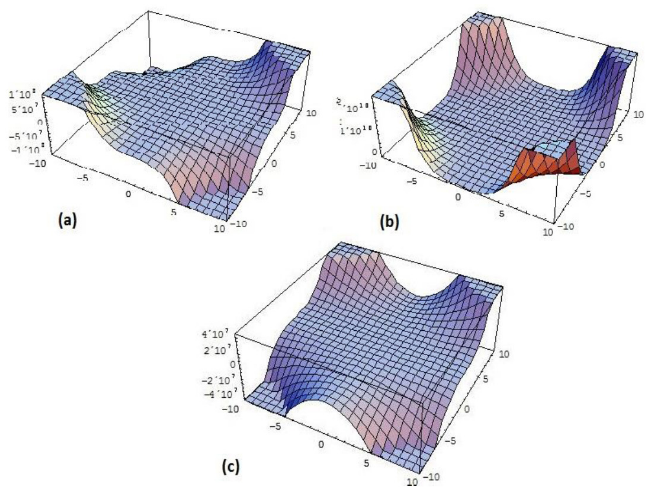

Figure 7

M-PO, (a)*MG*, (b)*LG*, (c)*SG* of *VPNTU [l, k]*.

6. Plotting and comparing M-Polynomial for *VPNTU[l, k]* and *VPNTO[l, k]*

The graphical representation of the M-Polynomial of *MG*, *LG* and *SG* of *VPNTU [l, k]* is given by Figure (7).

The graphical representation of the *M-PO* of *MG*, *LG* and *SG* of *VPNTO [l, k]* is given by Figure (8).

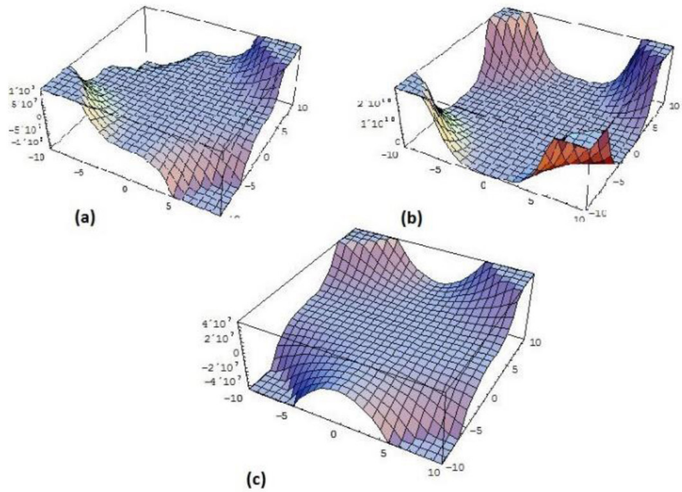

Figure 8

M-PO, (a) *MG*, (b)*LG*, (c), *SG* of *VPNTO [l, k]*.

7. MATLAB coding for *TI*

In this section, we provide MATLAB coding for the calculation of *TI* using M-polynomial and the relationships proved in Section (5).

The product connectivity *RI* from M-polynomial coding is computed as,

```
clear
clc
ns=input('number of sentence:');

A=zeros(ns,3);
m=input('enter m:');
n=input('enter n:');
    Delta=input('enter maximum degree of graph:');
    dlta=input('enter minimum degree of graph:');
```

```
syms m n
for c=1:ns
    for v=1:3
        if v==1
            fxy = input('tabe zarib:','s');
            A(c,v)=subs(fxy,[m,n],[1,1]);
        else
            A(c,v)=input('data: ');
        end
    end
end
A
    syms x y
    mGxy=0;
    for c=1:ns

            mGxy=mGxy+A(c,1)*x^A(c,2)*y^A(c,3);
    end
    mGxy

f=-Delta-dlta;
    B=zeros(ns,3);
    for c=1:ns
        for v=1:3
            if v==1
            B(c,v)=A(c,v);
            else
                B(c,v)=A(c,v)+f;
            end
        end
    end
    B
    FA=0;
    for c=ns:1:-1

            FA=FA+B(c,1)*x^B(c,2)*y^B(c,3);
        end
    FA;

    ZDX=zeros(ns,3);
    for c=1:ns
        for v=1:3
            if v==1
            ZDX(c,v)=B(c,v)*B(c,v+1);
            else
                ZDX(c,v)=B(c,v);
```

```
            end
        end
    end
    ZDX
    DX=0;
    for c=1:ns

            DX=ZDX(c,1)*x^ZDX(c,2)*y^ZDX(c,3)+DX;
        end
    DX=sqrt(DX)
    ZDY=zeros(ns,3);
    for c=1:ns
        for v=1:3
            if v==1
            ZDY(c,v)=B(c,v)*B(c,v+2);
            else
                ZDY(c,v)=B(c,v);
            end
        end
    end
    ZDY
    DY=0;
    for c=1:ns

            DY=ZDY(c,1)*x^ZDY(c,2)*y^ZDY(c,3)+DY;
        end
    DY=sqrt(DY)


ZDXDY=zeros(ns,3);
for c=1:ns
    for v=1:3
        if v==1
        ZDXDY(c,v)=A(c,v)*B(c,v+1)*B(c,v+2);
        else
            ZDXDY(c,v)=ZDX(c,v);
        end
    end
end
ZDXDY
DXDY=0;
for c=1:ns

        DXDY=ZDXDY(c,1)*x^ZDXDY(c,2)*y^ZDXDY(c,3)+DXDY;
    end
DXDY
HR1=sqrt(DXDY)
t=vpa(subs(HR1,[x,y],[1,1]))
D=1/t
```

8. Conclusion

This article presents new *RI* obtained through the use of M-polynomial calculations. Additionally, we apply M-polynomial and new *RI* to five classes of *VPNTU [l, k]* and *VPNTO [l, k]* and present graphical representations of the results in Figures (7) and (8). Our findings highlight the potential of these *TI* in predicting reactivity and other properties of other *CNT*, which could have significant implications for future research in this field. In future, one can also work on other *RI* from M-polynomial coding.

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