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Research Article

Verification of Some Topological Indices of *Y*-Junction Based Nanostructures by M-Polynomials

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The concept of M-polynomials determines the algebraic form of a system or network. It creates a structure into an algebraic equation and makes work easy to do on such a structure. This has diverse uses in different applied mathematics and as well as in engineering fields. In this study, we look closely at the abstract form of Y-shaped junctions. For the generic view of Y-shaped junctions, we developed some vertex-degree-based M-polynomials formulas. On Y-shaped junctions, we discussed some topological index-based concepts as well and verified the results available in the literature.

1. Introduction

The future of multiterminal networks and electronic appliances is possible by the building blocks made by nanotube junctions or branched nanotubes. There are many types of nanotube junctions serving nano-electronics, such as L, T, Y, and X. For the literature on the electrical properties of different junctions, we refer to see [1–3], its mechanical stability [4], conduction mechanism and transport phenomena [5], thermal rectification [6]. Instead of straight nanotubes, nanostructures developed using the nanotube junctions are anticipated to deliver much better in terms of mechanical properties. In order to create nanostructures, nanotubes are combined, their techniques, approaches, and succinct descriptions are available (see, for example, [7, 8]).

In this presented work, we will only consider discussing Y-type junctions of carbon nanotubes. It is obvious by name that Y-junctions are having the shape of Y-alphabet and are made by joining three nanotubes. These three nanotubes are joined on a point named as branching point as shown in Figure 1, which is itself comprised of hexagons and six heptagons. If the pattern of hexagons surrounds each heptagon with a pattern distributed symmetrically, and nanotubes are joined in the identical Y-shape, these types of Y-junctions are symmetric.

On the topology of nanotubes, Y-junctions may have further subtypes. For example, single-walled nanotubes have three types of geometries, chiral, zig-zag, and armchair. So developed Y-junctions are regarded as armchair carbon nanotube Y-junction. All these properties are available for multiwalled nanotubes. In 1991, the first nanotube was discovered [9], and after two years, the first structural topology of a Y-shaped junction was made by the authors of [10, 11] independently. The researchers in [12] experimentally observed these junctions in 1995. In [13, 14], the authors presented the idea of asymmetric and symmetric Y-shaped junctions, their constructions, their models, and their numerous variants. The applications and properties of novel structure Y-shaped junctions are presented in [15, 16].

The quantitative structure-property and activity relationships are solely concerned with the forecasting of bioactivities and chemical or biological structure properties. Topological indices and physicochemical properties are used to aid prediction in this method. There is a significant body

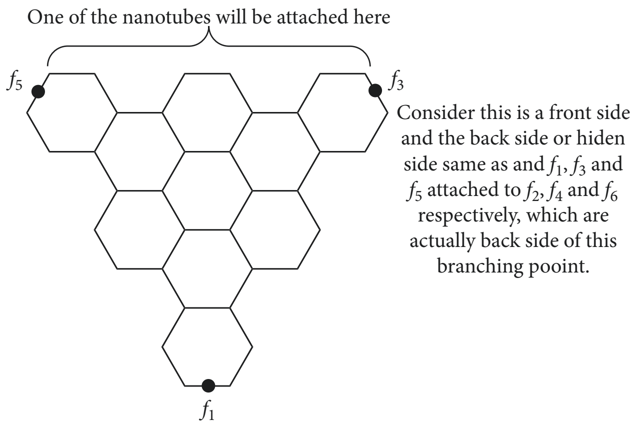

Figure 1: A branching point $Y(6,6)$.

of literature related to the topological descriptors of chemical structure, which can be found in [17]; for example, the authors of [18] discussed some various types of nanotubes and nanostructures, the authors of [19, 20] studied some chemical networks like honeycomb networks and nanotubes, and different structures made by basic operations of linear algebras are discussed in [21]. For more studies on this topic, we suggest to refer [22–25]. For some relevant topics, we offer the literature found in [26–29]. In the following section of this paper, there are some basic formulas for predicting the physical properties of a network and system.

Definition 1. Hosoya polynomials, the famous most and very first, were introduced in 1988, and in 2015, a modified polynomial, also known as M-polynomial, is introduced by [30]. This form of the polynomial has a closed relationship to degree-based topological indices. Topological indices from M-polynomials of a graph may be obtained using a specific format. This M-polynomial may be defined as follows:

$$\Pi(\chi; x, y) = \sum_{i \le j} \alpha_{i,j}(\chi) x^i y^j, \tag{1}$$

where $\alpha_{i,j}(\chi)$ is considered as the size of graph χ given that $i \le j$.

Definition 2 (see [31, 32]). The first Zagreb index of graph χ is

$$M_1(\chi) = \sum_{uv \in E(\chi)} (d(u) + d(v)). \tag{2}$$

Definition 3 (see [31, 32]). The second Zagreb index of graph χ is

$$M_2(\chi) = \sum_{uv \in E(\chi)} (d(u) \cdot d(v)). \tag{3}$$

Definition 4 (see [33]). The M-polynomial of the first and the second Zagreb indices is

$$\prod_{M_1}(\chi) = \left(D_x + D_y\right)(\Pi(\chi; x, y)), \tag{4}$$

$$\prod_{M_2}(\chi) = \left(D_x + D_y\right)(\Pi(\chi; x, y)). \tag{5}$$

Definition 5 (see [31–33]). The general Randić index and its M-polynomials are

$$R_\alpha(\chi) = \sum_{uv \in E(\chi)} (d(u) \cdot d(v))^\alpha, \tag{6}$$

$$\prod_{R_\alpha}(\chi) = \left(D_x^\alpha D_y^\alpha\right)(\Pi(\chi; x, y)). \tag{7}$$

Definition 6 (see [33]). The operators are defined as follows:

$$D_x(\Pi(\chi; x, y)) = x \frac{\partial(\Pi(\chi; x, y))}{\partial x}, \tag{8}$$

$$D_y(\Pi(\chi; x, y)) = y \frac{\partial(\Pi(\chi; x, y))}{\partial y}, \tag{9}$$

$$S_x(\Pi(\chi; x, y)) = \int_0^x \frac{(\Pi(\chi; z, y))}{z} \mathrm{d}z, \tag{10}$$

$$S_y(\Pi(\chi; x, y)) = \int_0^y \frac{(\Pi(\chi; x, z))}{z} \mathrm{d}z. \tag{11}$$

The primary goal or participation of this study work is to investigate some vertex-degree-based M-polynomials of Y-shaped junctions and their variants, as well as some comprehensive applications of the theoretical and practical approach of Y-shaped junctions and their variants. We will investigate the structure of Y-shaped junctions and their variants in the following section. We will also present some key findings on the vertex-degree-based M-polynomials of Y-shaped junctions and their variants. Finally, we will reach a conclusion. There would be some interesting and important references to literature. To entice the reader to investigate Y-shaped junctions and their variants, vertex-degree-based M-polynomials, topological index are discussed in this research work. Furthermore, we also consider to discuss the applications for the Y-shaped junctions and their variants.

2. *Y*-Junction Graphs and Methodology of Presented Work

For the aims of computation, the structures of the Y-junction are transformed in the vertex-edge graph, and for this, we follow the methodology presented in [34, 35]. The vertex-degree-based edge types are measured after getting the molecular graphs of junctions and their variants. These vertex-degree-based specifications of edges are necessary tools to compute our main results.

The Y-junctions investigated in this study are formed by the covalent connectivity of three armchair single-walled carbon nanotubes of finite length, and these nanotubes crossed at an angle of 120 degrees and are determined by a chiral vector (n, n).

Let $k \geq 2$ for the parameter $n = 2k$ are integers and $m \geq 1$. A Y-shaped junction graph $J_m(n, n)$ is assembled by making an armchair $Y(n, n)$, which is called as branching point, and three carbon nanotubes $T_m(n, n)$ of same length of m-layers of hexagons. It has $6k^2 + 18k + 24mk + 6$ number of vertices, and the edges are $9k^2 + 21k + 36mk + 9$ in total. It has $6k^2 + 6k + 24mk + 6$, degree three vertices, and only $12k$ degree 2 vertices. Each nanotube comprises of $4mk$ faces of hexagons while branching point comprises of $3k^2 - 3k + 5$ faces. In these faces, $3k^2 - 3k - 4$ hexagons, six heptagons, and only three faces were nanotubes joined with branching point.

The notation $J_m(n, n)$ is referred as graph of Y-shaped junction, and it contained no vertex of one degree. The notation $I' J_m(n, n)$ is an extension of graph of Y-shaped junction $J_m(n, n)$ as shown in Figure 2. This graph $(I' J_m(n, n))$ appears when one of the three nanotubes has exactly $4k$ degree one vertices. The total number of vertices and edges of $I' J_m(n, n)$ are $24mk + 6k^2 + 22k + 6$ and $36mk + 9k^2 + 25k + 9$, accordingly. The graph with notation $I'' J_m(n, n)$ is another extension of $J_m(n, n)$ junction graph. It contains $36mk + 9k^2 + 29k + 9$ edges and $24mk + 6k^2 + 26k + 6$ vertices. This graph is obtained by having $8k$ degree one vertices on any two nanotubes of $J_m(n, n)$. In total, $12k$ degree one vertices attaching to all three nanotubes of $J_m(n, n)$ made another variant Y-junction, and it is known as $I''' J_m(n, n)$. This newly developed graph contains $36mk + 9k^2 + 33k + 9$ edges and $24mk + 6k^2 + 30k + 6$ vertices.

The structure shown in Figure 1 is a front view of branching point $Y(n, n)$ with $n = 6$. There are three sides where armchair carbon nanotubes $T_m(n, n)$ with different lengths, which is $m \geq 1$, will be attached. The structure shown in the Figure 2 is a variant of Y-junction having $4k$ pendent or one degree vertices, and the notation used is $I' J_m(n, n)$. In the same figure, a place on a single nanotube is pointed where the extension of one degree $4k$, $8k$, and $12k$ vertices can be attached for different variants of Y-junctions, and these variants are denoted as $I' J_m(n, n)$, $I'' J_m(n, n)$, and $I''' J_m(n, n)$, respectively. Without any one degree vertex, there will be original Y-junction of notation $J_m(n, n)$.

Some vertex-degree-based M-polynomials for Y-junction and its all variants are as follows.

Theorem 1. *Let $J_m(n, n)$ be a structure of Y-type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $\Pi(J_m(n, n); x, y)$ is the general M-polynomials for $J_m(n, n)$. Then,*

$$\Pi(J_m(n, n); x, y) = 6kx^2y^2 + 12kx^2y^3 + \left(9k^2 + 3k + 36mk + 9\right)x^3y^3. \tag{12}$$

Proof. From Figure 2, which is the construction for the structure of Y-type junction, we can observe that there are three edge partitions based on the degree of end vertices of each edge that is defined as follows:

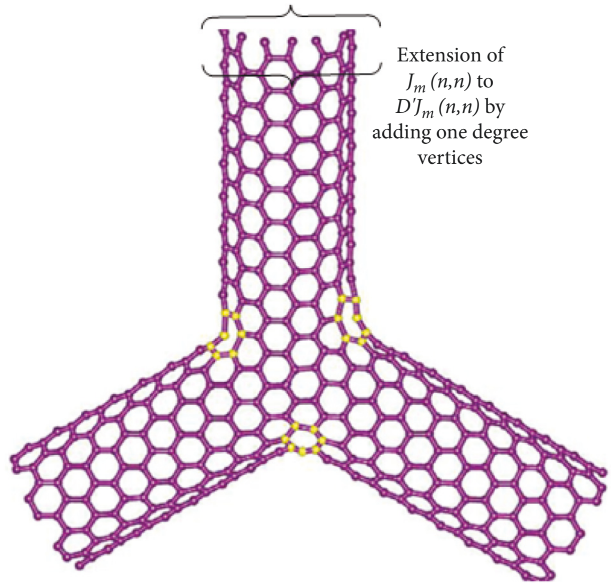

Figure 2: A variant of Y-junction $I'J_m(n, n)$.

$$e_{2,2} = \{uv \in E(J_m(n, n)) : d(u) = d(v) = 2\}, \tag{13}$$

$$te_{2,3} = \{uv \in E(J_m(n, n)) : d(u) = 2, d(v) = 3\}, \tag{14}$$

$$e_{3,3} = \{uv \in E(J_m(n, n)) : d(u) = d(v) = 3\}. \tag{15}$$

The numbers of these edge types are $|e_{2,2}| = 6k$, $|e_{2,3}| = 12k$, and $|e_{3,3}| = 9k^2 + 3k + 36mk + 9$. Then, from the Definition 1, the M-polynomial of $J_m(n, n)$ can be found as

$$\begin{aligned}\Pi(J_m(n, n); x, y) &= \sum_{i \leq j} m_{i,j}(J_m(n, n)) x^i y^j \\ &= 6kx^2y^2 + 12kx^2y^3 \\ &\quad + \left(9k^2 + 3k + 36mk + 9\right)x^3y^3.\end{aligned} \tag{16}$$

□

Lemma 1. *Let $J_m(n, n)$ be a structure of Y-type junction with $k \geq 2$, $n = 2k$, $m \geq 1$, $D_x(\Pi(J_m(n, n); x, y))$ and $D_y(\Pi(J_m(n, n); x, y))$ are the differential operators for $J_m(n, n)$. Then,*

$$D_x(\Pi(J_m(n, n); x, y)) = 12kx^2y^2 + 24kx^2y^3 + \left(27k^2 + 9k + 108mk + 27\right)x^3y^3, \tag{17}$$

$$D_y(\Pi(J_m(n, n); x, y)) = 12kx^2y^2 + 36kx^2y^3 + \left(27k^2 + 9k + 108mk + 27\right)x^3y^3. \tag{18}$$

Proof. In this proof, we will provide an example of the usage of differential operators. Differentiating the equation given in the proof of Theorem 1 with respect to variable x and times the result with the same variable. We will have the required result of the operator $D_x(\Pi(J_m(n,n);x,y))$, for the structure of the Y-type junction which is $J_m(n,n)$.

$$\begin{aligned}D_x(\Pi(J_m(n,n);x,y)) &= x\frac{\partial \Pi(J_m(n,n))}{\partial x}\\ &= x\frac{\partial}{\partial x}\left((6k)x^2y^2+(12k)x^2y^3+\left(9k^2+3k+36mk+9\right)x^3y^3\right)\\ &= x\left((12k)xy^2+(24k)xy^3+\left(27k^2+9k+108mk+27\right)x^2y^3\right)\\ &= 12kx^2y^2+24kx^2y^3+\left(27k^2+9k+108mk+27\right)x^3y^3.\end{aligned} \tag{19}$$

Similarly, by differentiating the equation given in the proof of Theorem 1 with respect to variable y and times the result with the same variable, we will have the required result of the operator $D_y(\Pi(J_m(n,n);x,y))$, for the structure of Y-type junction which is $J_m(n,n)$.

$$\begin{aligned}D_y(\Pi(J_m(n,n);x,y)) &= y\frac{\partial \Pi(J_m(n,n))}{\partial y}\\ &= y\frac{\partial}{\partial y}\left((6k)x^2y^2+(12k)x^2y^3+\left(9k^2+3k+36mk+9\right)x^3y^3\right)\\ &= y\left((12k)x^2y+(36k)x^2y^2+\left(27k^2+9k+108mk+27\right)x^3y^2\right)\\ &= 12kx^2y^2+36kx^2y^3+\left(27k^2+9k+108mk+27\right)x^3y^3.\end{aligned} \tag{20}$$

□

Lemma 2. *Let $J_m(n,n)$ be a structure of Y-type junction with $k\geq 2$, $n=2k$, $m\geq 1$, $S_x(\Pi(J_m(n,n);x,y))$ and $S_y(\Pi(J_m(n,n);x,y))$ are the integral operators for $J_m(n,n)$. Then,*

$$S_x(\Pi(J_m(n,n);x,y)) = 3kx^2y^2+6kx^2y^3+\left(3k^2+k+18mk+3\right)x^3y^3, \tag{21}$$

$$S_y(\Pi(J_m(n,n);x,y)) = 2kxy^3+3kxy^4+\frac{3\left(3k^2+k+18mk+3\right)}{4}xy^4. \tag{22}$$

Proof. In this proof, we will provide an example of the usage of integral operators. Introducing a new parameter in the place of a variable x, and integrating the equation given in the proof of Theorem 1 with respect to the same variable, let say z and times the result with the same variable. We will have the required result of the operator $S_x(\Pi(J_m(n,n);x,y))$, for the structure of the Y-type junction which is $J_m(n,n)$.

$$\begin{aligned}S_x(\Pi(J_m(n,n);x,y)) &= \int_0^x \frac{\Pi(J_m(n,n);z,y)}{z}\mathrm{d}z\\ &= \int_0^x \frac{1}{z}\left((6k)z^2y^2+(12k)z^2y^3+\left(9k^2+3k+36mk+9\right)z^3y^3\right)\mathrm{d}z\\ &= \int_0^x (6k)zy^2+\int_0^x (12k)zy^3+\int_0^x\left(9k^2+3k+36mk+9\right)z^2y^3\mathrm{d}z\\ &= (6k)\frac{z^2}{2}y^2\Big|_0^x+(12k)\frac{z^2}{2}y^3\Big|_0^x+\left(9k^2+3k+36mk+9\right)\frac{z^3}{3}y^3\Big|_0^x\\ &= 3kx^2y^2+6kx^2y^3+\left(3k^2+k+18mk+3\right)x^3y^3.\end{aligned} \tag{23}$$

Similarly, by introducing a new parameter in the place of variable y and integrating the equation given in the proof of Theorem 1 with respect to the same variable, let say z and times the result with same variable, we will have the required result of operator $S_y(\Pi(J_m(n,n);x,y))$, for the structure of Y-type junction which is $J_m(n,n)$.

$$
\begin{aligned}
S_y(\Pi(J_m(n,n);x,y)) &= \int_0^y \frac{\Pi(J_m(n,n);x,z)}{z}\mathrm{d}z \\
&= \int_0^y \frac{1}{z}\left((6k)x^2z^2 + (12k)x^2z^3 + \left(9k^2 + 3k + 36mk + 9\right)x^3z^3\right)\mathrm{d}z \\
&= \int_0^y (6k)xz^2 + \int_0^y (12k)xz^3 + \int_0^y \left(9k^2 + 3k + 36mk + 9\right)x^2z^3\mathrm{d}z \\
&= (6k)x\frac{z^3}{3}\bigg|_0^y + (12k)x\frac{z^4}{4}\bigg|_0^y + \left(9k^2 + 3k + 36mk + 9\right)x\frac{z^4}{4}\bigg|_0^y \\
&= 2kxy^3 + 3kxy^4 + \frac{3\left(3k^2 + k + 18mk + 3\right)}{4}xy^4.
\end{aligned}
\tag{24}
$$

□

Theorem 2. *Let $J_m(n,n)$ be a structure of Y-type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $\prod_{M_1}(J_m(n,n);x,y)$ is the first Zagreb M-polynomials for $J_m(n,n)$. Then,*

$$
\begin{aligned}
\prod_{M_1}(J_m(n,n)) = 24kx^2y^2 + 60k + x^2y^3 \\
+\left(54k^2 + 18k + 216mk + 54\right)x^3y^3.
\end{aligned}
\tag{25}
$$

Proof. A method to compute the first Zagreb M-polynomial, given in the equation (4) of Definition 4, and this methodology is derived from the basic formula of the first Zagreb index given in the equation (2) of Definition 2. Now, by using the differential operator of $J_m(n,n)$ defined in the Lemma 1 and applying on the equation (4), we will have the required result of first Zagreb M-polynomial of $J_m(n,n)$, which is computed as follows:

$$
\begin{aligned}
\prod_{M_1}(J_m(n,n)) &= \left(D_x + D_y\right)(\Pi(J_m(n,n))) \\
&= D_x(\Pi(J_m(n,n))) + D_y(\Pi(J_m(n,n))) \\
&= (12k)x^2y^2 + (24k)x^2y^3 + \left(27k^2 + 9k + 108mk + 27\right)x^3y^3 \\
&\quad + (12k)x^2y^2 + (36k)x^2y^3 + \left(27k^2 + 9k + 108mk + 27\right)x^3y^3 \\
&= 24kx^2y^2 + 60kx^2y^3 + \left(54k^2 + 18k + 216mk + 54\right)x^3y^3.
\end{aligned}
\tag{26}
$$

□

Theorem 3. *Let $J_m(n,n)$ be a structure of Y-type junction with $k \geq 2$, $n = 2k$, $m \geq 1$, and $\prod_{M_2}(J_m(n,n);x,y)$ is the second Zagreb M-polynomials for $J_m(n,n)$. Then,*

$$
\begin{aligned}
\prod_{M_2}(J_m(n,n)) = 24kx^2y^2 + 72kx^2y^3 \\
+ 3\left(27k^2 + 9k + 108mk + 27\right)x^3y^3.
\end{aligned}
\tag{27}
$$

Proof. A method to compute the second Zagreb M-polynomial, given in the equation (5) of Definition 4, and this methodology is derived from the basic formula of the second Zagreb index given in the equation (3) of Definition 3. Now using the differential operator of $J_m(n,n)$, defined in the Lemma 1 and applying it on the equation (5), we will have the required result of the second Zagreb M-polynomial of $J_m(n,n)$, which is computed as follows:

$$
\begin{aligned}
\prod_{M_2}(J_m(n,n)) &= \left(D_xD_y\right)(\Pi(J_m(n,n))) \\
&= D_x\left((12k)x^2y^2 + (36k)x^2y^3 + \left(27k^2 + 9k + 108mk + 27\right)x^3y^3\right) \\
&= 24kx^2y^2 + 72kx^2y^3 + 3\left(27k^2 + 9k + 108mk + 27\right)x^3y^3.
\end{aligned}
\tag{28}
$$

□

Theorem 4. *Let $J_m(n,n)$ be a structure of Y-type junction with $k\geq 2$, $n=2k$, $m\geq 1$, and $\Pi_{R_\alpha}(J_m(n,n);x,y)$ is the general Randić M-polynomials for $J_m(n,n)$. Then,*

$$\prod_{R_\alpha}(J_m(n,n)) = 4^\alpha(6k)x^2y^2 + 6^\alpha(12k)x^2y^3 + 9^\alpha\left(9k^2+3k+36mk+9\right)x^3y^3. \tag{29}$$

Proof. A method to compute the generalized Randić M-polynomial is given in equation (7) of Definition 5, and this methodology is derived from the basic formula of the generalized Randić index as given in equation (6) of Definition 5. Now, by using the generalized view of differential operators of $J_m(n,n)$, defined in the Lemma 1, and applying it on equation (7), we will have the required result of generalized Randić M-polynomial of $J_m(n,n)$, which is computed as follows:

$$\begin{aligned}\prod_{R_\alpha}(J_m(n,n)) &= \left(D_x^\alpha D_y^\alpha\right)(\Pi(J_m(n,n)))\\ &= \left(D_x^\alpha D_y^\alpha\right)\left((6k)x^2y^2+(12k)x^2y^3+\left(9k^2+3k+36mk+9\right)x^3y^3\right)\\ &= D_x^\alpha\left(2^\alpha(6k)x^2y^2+3^\alpha(12k)x^2y^3+3^\alpha\left(9k^2+3k+36mk+9\right)x^3y^3\right)\\ &= 4^\alpha(6k)x^2y^2+6^\alpha(12k)x^2y^3+9^\alpha\left(9k^2+3k+36mk+9\right)x^3y^3.\end{aligned} \tag{30}$$

□

3. $I'J_m(n,n)$ Structure of Y-Second Type Junction

Theorem 5. *Let $I'J_m(n,n)$ be a structure of Y-second type junction with $k\geq 2$, $n=2k$, $m\geq 1$ and $\prod(I'J_m(n,n);x,y)$ is the general M-polynomials for $I'J_m(n,n)$. Then,*

$$\Pi(I'J_m(n,n);x,y) = 4kxy^3+4kx^2y^2+8kx^2y^3 + \left(9k^2+9k+36mk+9\right)x^3y^3. \tag{31}$$

Proof. From Figure 2, which is the construction for the structure of Y-second type junction, we can observe that there are four edge partitions based on the degree of end vertices of each edge that is defined as

$$\begin{aligned}e_{1,3} &= \{uv\in E(I'J_m(n,n)) : d(u)=1,\ d(v)=3\},\\ e_{2,2} &= \{uv\in E(I'J_m(n,n)) : d(u)=d(v)=2\},\end{aligned} \tag{32}$$

$$e_{2,3} = \{uv\in E(I'J_m(n,n)) : d(u)=2,\ d(v)=3\}, \tag{33}$$

$$e_{3,3} = \{uv\in E(I'J_m(n,n)) : d(u)=d(v)=3\}. \tag{34}$$

The numbers of these edge types are $|e_{1,3}|=4k$, $|e_{2,2}|=4k$, $|e_{2,3}|=8k$ and $|e_{3,3}|=9k^2+9k+36mk+9$. Then from the Definition 1, the M-polynomial of $I'J_m(n,n)$ can be found as

$$\prod(I'J_m(n,n);x,y) = \sum_{i\leq j} m_{i,j}(I'J_m(n,n))x^iy^j = 4kxy^3+4kx^2y^2+8kx^2y^3+\left(9k^2+9k+36mk+9\right)x^3y^3. \tag{35}$$

□

Lemma 3. *Let $I'J_m(n,n)$ be a structure of Y-second type junction with $k\geq 2$, $n=2k$, $m\geq 1$, $D_x(\Pi(I'J_m(n,n);x,y))$ and $D_y(\Pi(I'J_m(n,n);x,y))$ are the differential operators for $I'J_m(n,n)$. Then,*

$$D_x(\Pi(I'J_m(n,n);x,y)) = 4kxy^3+8kx^2y^2+16kx^2y^3+\left(27k^2+27k+108mk+27\right)x^3y^3, \tag{36}$$

$$D_y(\Pi(I'J_m(n,n);x,y)) = 12kxy^3+8kx^2y^2+24kx^2y^3+\left(27k^2+27k+108mk+27\right)x^3y^3. \tag{37}$$

Proof. In this proof, we will provide an example for the usage of differential operators. By differentiating the equation given in the proof of Theorem 5 with respect to variable x and times the result with same variable, we will have the required result of operator $D_x(\Pi(I'J_m(n,n);x,y))$, for the structure of Y-type junction which is $I'J_m(n,n)$.

$$\begin{aligned}
&D_x\left(\Pi\left(I'J_m(n,n);x,y\right)\right)\\
&= x\frac{\partial \Pi\left(I'J_m(n,n)\right)}{\partial x}\\
&= x\frac{\partial}{\partial x}\left((4k)xy^3+(4k)x^2y^2+(8k)x^2y^3+\left(9k^2+9k+36mk+9\right)x^3y^3\right)\\
&= x|\left((4k)xy^3+(8k)x^2y^2+(16k)x^2y^3+\left(27k^2+27k+108mk+27\right)x^3y^3\right)\\
&= 4kxy^3+8kx^2y^2+16kx^2y^3+\left(27k^2+27k+108mk+27\right)x^3y^3.
\end{aligned} \tag{38}$$

Similarly, by differentiating the equation given in the proof of Theorem 5 with respect to variable y and times the result with same variable, we will have the required result of operator $D_y\left(\Pi\left(I'J_m(n,n);x,y\right)\right)$, for the structure of Y-type junction which is $I'J_m(n,n)$.

$$\begin{aligned}
&D_y\left(\Pi\left(I'J_m(n,n);x,y\right)\right)\\
&= y\frac{\partial \Pi\left(I'J_m(n,n)\right)}{\partial y}\\
&= y\frac{\partial}{\partial y}\left((4k)xy^3+(4k)x^2y^2+(8k)x^2y^3+\left(9k^2+9k+36mk+9\right)x^3y^3\right)\\
&= y\left((12k)xy^3+(8k)x^2y^2+(24k)x^2y^3+\left(27k^2+27k+108mk+27\right)x^3y^3\right)\\
&= 12kxy^3+8kx^2y^2+24kx^2y^3+\left(27k^2+27k+108mk+27\right)x^3y^3.
\end{aligned} \tag{39}$$

□

Lemma 4. *Let $I'J_m(n,n)$ be a structure of Y-second type junction with $k\geq 2$, $n=2k$, $m\geq 1$, $S_x\left(\Pi\left(I'J_m(n,n);x,y\right)\right)$ and $S_y\left(\Pi\left(I'J_m(n,n);x,y\right)\right)$ are the integral operators for $I'J_m(n,n)$. Then,*

$$S_x\left(\Pi\left(I'J_m(n,n);x,y\right)\right)=4kxy^3+2kx^2y^2+4kx^2y^3+\left(3k^2+3k+18mk+3\right)x^3y^3, \tag{40}$$

$$S_y\left(\Pi\left(I'J_m(n,n);x,y\right)\right)=\frac{4k}{3}xy^3+2kx^2y^2+\frac{8k}{3}x^2y^3+\left(3k^2+3k+18mk+3\right)x^3y^3. \tag{41}$$

Proof. In this proof, we will provide an example for the usage of integral operators. Introducing a new parameter in the place of variable x, and integrating the equation given in the proof of Theorem 5 with respect to the same variable, let say z and times the result with the same variable. We will have the required result of operator $S_x\left(\Pi\left(I'J_m(n,n);x,y\right)\right)$, for the structure of Y-type junction which is $I'J_m(n,n)$.

$$
\begin{aligned}
&S_x(\Pi(I'J_m(n,n);x,y))\\
&= \int_0^x \frac{\Pi(J_m(n,n);z,y)}{z}\mathrm{d}z\\
&= \int_0^x \frac{1}{z}\left((4k)zy^3 + (4k)z^2y^2 + (8k)z^2y^3 + \left(9k^2 + 9k + 36mk + 9\right)z^3y^3\right)\mathrm{d}z\\
&= \int_0^x (4k)y^3 dz + \int_0^x (4k)zy^2 dz + \int_0^x (8k)zy^3 dz + \int_0^x \left(9k^2 + 9k + 36mk + 9\right)z^2y^3\mathrm{d}z\\
&= (4k)zy^3|_0^x + (4k)z^2y^2|_0^x + (8k)z^2y^3|_0^x + \left(9k^2|_0^x + 9k + 36mk + 9\right)z^3y^3|_0^x (6k)\frac{z^2}{2}y^2\Big|_0^x\\
&+ (12k)\frac{z^2}{2}y^3|_0^x + \left(9k^2 + 3k + 36mk + 9\right)\frac{z^3}{3}y^3|_0^x\\
&= 4kxy^3 + 2kx^2y^2 + 4kx^2y^3 + \left(3k^2 + 3k + 18mk + 3\right)x^3y^3.
\end{aligned} \tag{42}
$$

Similarly, introducing a new parameter in the place of variable y, and integrating the equation given in the proof of Theorem 5 with respect to the same variable, let say z and times the result with the same variable. We will have the required result of operator $S_y(\Pi(I'J_m(n,n);x,y))$, for the structure of the Y-type junction which is $I'J_m(n,n)$.

$$
\begin{aligned}
S_y(\Pi(I'J_m(n,n);x,y)) &= \int_0^y \frac{\Pi(J_m(n,n);x,z)}{z}\mathrm{d}z\\
&= \int_0^y \frac{1}{z}\left((4k)xz^3 + (4k)x^2z^2 + (8k)x^2z^3 + \left(9k^2 + 9k + 36mk + 9\right)x^3z^3\right)\mathrm{d}z\\
&= \int_0^y (4k)xz^2\mathrm{d}z + \int_0^y (4k)x^2z\mathrm{d}z + \int_0^y (8k)x^2z^2\mathrm{d}z + \int_0^y \left(9k^2 + 9k + 36mk + 9\right)x^3z^2\mathrm{d}z\\
&= (4k)xz^3|_0^y + (4k)x^2z^2|_0^y + (8k)x^2z^3|_0^y + \left(9k^2|_0^y + 9k + 36mk + 9\right)x^3z^3|_0^y\\
&= \frac{4k}{3}xy^3 + 2kx^2y^2 + \frac{8k}{3}x^2y^3 + \left(3k^2 + 3k + 18mk + 3\right)x^3y^3.
\end{aligned} \tag{43}
$$

□

Theorem 6. *Let $J_m(n,n)$ be a structure of Y-second type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $\Pi_{M_1}(I'J_m(n,n);x,y)$ is the first Zagreb M-polynomials for $I'J_m(n,n)$. Then*

$$
\begin{aligned}
\prod_{M_1}(I'J_m(n,n)) &= 16kxy^3 + 16kx^2y^2 + 40kx^2y^3\\
&\quad + \left(54k^2 + 54k + 216mk + 54\right)x^3y^3.
\end{aligned} \tag{44}
$$

Proof. A method to compute the first Zagreb M-polynomial is given in equation (4) of Definition 4, and this methodology is derived from the basic formula of the first Zagreb index given as shown in equation (2) of Definition 2. Now, by using the differential operator of $I'J_m(n,n)$, defined in the Lemma 3, and applying it to equation (4), we will have the required result of the first Zagreb M-polynomial of $I'J_m(n,n)$, which is computed as given follows:

$$\begin{aligned}\prod_{M_1}(I'J_m(n,n)) &= \left(D_x + D_y\right)\left(\Pi\left(I'J_m(n,n)\right)\right)\\ &= D_x\left(\Pi\left(I'J_m(n,n)\right)\right) + D_y\left(\Pi\left(I'J_m(n,n)\right)\right)\\ &= (4k)xy^3 + (8k)x^2y^2 + (16k)x^2y^3 + \left(27k^2 + 27k + 108mk + 27\right)x^3y^3 + (12k)xy^3\\ &\quad + (8k)x^2y^2 + (24k)x^2y^3 + \left(27k^2 + 27k + 108mk + 27\right)x^3y^3\\ &= 16kxy^3 + 16kx^2y^2 + 40kx^2y^3 + \left(54k^2 + 54k + 216mk + 54\right)x^3y^3.\end{aligned} \tag{45}$$

□

Theorem 7. *Let $J_m(n,n)$ be a structure of Y-second type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $\Pi_{M_2}(I'J_m(n,n); x, y)$ is the second Zagreb M-polynomials for $I'J_m(n,n)$. Then,*

$$\prod_{M_2}(I'J_m(n,n)) = 12kxy^3 + 16kx^2y^2 + 48kx^2y^3 + \left(81k^2 + 81k + 324mk + 81\right)x^3y^3. \tag{46}$$

Proof. A method to compute the second Zagreb M-polynomial is given in equation (5) of Definition 4, and this methodology is derived from the basic formula of the second Zagreb index given in equation (3) of Definition 3. Now, by using the differential operator of $I'J_m(n,n)$, defined in the Lemma 3 and applying it to equation (5), we will have the required result of the second Zagreb M-polynomial of $I'J_m(n,n)$, which is computed as follows:

$$\begin{aligned}\prod_{M_2}(I'J_m(n,n)) &= \left(D_xD_y\right)\left(\Pi\left(I'J_m(n,n)\right)\right)\\ &= D_x\left((12k)xy^3 + (8k)x^2y^2 + (24k)x^2y^3 + \left(27k^2 + 27k + 108mk + 27\right)x^3y^3\right)\\ &= 12kxy^3 + 16kx^2y^2 + 48kx^2y^3 + \left(81k^2 + 81k + 324mk + 81\right)x^3y^3.\end{aligned} \tag{47}$$

□

Theorem 8. *Let $J_m(n,n)$ be a structure of Y-second type junction with $k \geq 2$, $n = 2k$, $m \geq 1$, and $\Pi_{R_\alpha}(I'J_m(n,n); x, y)$ is the general Randić M-polynomials for $I'J_m(n,n)$. Then,*

$$\prod_{R_\alpha}(I'J_m(n,n)) = 3^\alpha(4k)xy^3 + 2^{2\alpha}(4k)x^2y^2 + 6^\alpha(8k)x^2y^3 + 3^{2\alpha}\left(9k^2 + 9k + 36mk + 9\right)x^3y^3. \tag{48}$$

Proof. A method to compute the generalized Randić M-polynomial is given in the following equation of Definition 5, and this methodology is derived from the basic formula of the generalized Randić index as given in equation (6) of Definition 5. Now, by using the generalized view of differential operators of $I'J_m(n,n)$, defined in the Lemma 3, and applying it to equation (7), we will have the required result of generalized Randić M-polynomial of $I'J_m(n,n)$, which is computed as follows:

$$\begin{aligned}\prod_{R_\alpha}(I'J_m(n,n)) &= \left(D_x^\alpha D_y^\alpha\right)\left(\Pi\left(I'J_m(n,n)\right)\right)\\ &= \left(D_x^\alpha D_y^\alpha\right)\left(4kxy^3 + 4kx^2y^2 + 8kx^2y^3 + \left(9k^2 + 9k + 36mk + 9\right)x^3y^3\right)\\ &= 3^\alpha(4k)xy^3 + 2^{2\alpha}(4k)x^2y^2 + 6^\alpha(8k)x^2y^3 + 3^{2\alpha}\left(9k^2 + 9k + 36mk + 9\right)x^3y^3.\end{aligned} \tag{49}$$

□

4. $I''J_m(n,n)$ Structure of Y-Third Type Junction

Theorem 9. *Let $I''J_m(n,n)$ be a structure of Y-third type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $\Pi(I''J_m(n,n); x, y)$ is the general M-polynomials for $I''J_m(n,n)$. Then,*

$$\Pi(I''J_m(n,n); x, y) = 8kxy^3 + 2kx^2y^2 + 4kx^2y^3 + \left(9k^2 + 15k + 36mk + 9\right)x^3y^3. \tag{50}$$

Proof. From Figure 2, which is the construction for the structure of the Y-second type junction, we can observe that there are four edge partitions based on the degree of end vertices of each edge that is defined as follows:

$$e_{1,3} = \{uv \in E(I''J_m(n,n)) \colon d(u) = 1,\ d(v) = 3\},\quad e_{2,2} = \{uv \in E(I''J_m(n,n)) \colon d(u) = d(v) = 2\}, \tag{51}$$

$$e_{2,3} = \{uv \in E(I''J_m(n,n)) \colon d(u) = 2, d(v) = 3\}, \tag{52}$$

$$e_{3,3} = \{uv \in E(I''J_m(n,n)) \colon d(u) = d(v) = 3\}. \tag{53}$$

The numbers of these edge types are $|e_{1,3}| = 8k$, $|e_{2,2}| = 2k$, $|e_{2,3}| = 4k$, and $|e_{3,3}| = 9k^2 + 15k + 36mk + 9$. Then, from the Definition 1, the M-polynomial of $I''J_m(n,n)$ can be found as

$$\begin{aligned}\Pi(I''J_m(n,n); x, y) &= \sum_{i\le j} m_{i,j}(I''J_m(n,n))x^i y^j \\ &= 8kxy^3 + 2kx^2y^2 + 4kx^2y^3 + \left(9k^2 + 15k + 36mk + 9\right)x^3y^3.\end{aligned} \tag{54}$$

□

Lemma 5. *Let $I''J_m(n,n)$ be a structure of Y-third type junction with $k \ge 2$, $n = 2k$, $m \ge 1$, $D_x(\Pi(I''J_m(n,n); x, y))$ and $D_y(I''\Pi(J_m(n,n); x, y))$ are the differential operators for $I''J_m(n,n)$. Then,*

$$D_x(\Pi(I''J_m(n,n); x, y)) = 8kxy^3 + 4kx^2y^2 + 8kx^2y^3 + \left(27k^2 + 45k + 108mk + 27\right)x^3y^3, \tag{55}$$

$$D_y(\Pi(I''J_m(n,n); x, y)) = 24kxy^3 + 4kx^2y^2 + 12kx^2y^3 + \left(27k^2 + 45k + 108mk + 27\right)x^3y^3. \tag{56}$$

Proof. In this proof, we will provide an example for the usage of differential operators. By differentiating the equation given in the proof of Theorem 9 with respect to variable x and times the result with the same variable, we will have the required result of the operator $D_x(\Pi(I''J_m(n,n); x, y))$, for the structure of Y-type junction, which is $I''J_m(n,n)$.

$$\begin{aligned}D_x(\Pi(I''J_m(n,n); x, y)) &= x\frac{\partial \Pi(I''J_m(n,n))}{\partial x} \\ &= x\frac{\partial}{\partial x}\left((8k)xy^3 + (2k)x^2y^2 + (4k)x^2y^3 + \left(9k^2 + 15k + 36mk + 9\right)x^3y^3\right) \\ &= x\left((8k)y^3 + (4k)xy^2 + (8k)xy^3 + \left(27k^2 + 45k + 108mk + 27\right)x^2y^3\right) \\ &= 8kxy^3 + 4kx^2y^2 + 8kx^2y^3 + \left(27k^2 + 45k + 108mk + 27\right)x^3y^3.\end{aligned} \tag{57}$$

Similarly, by differentiating the equation given in the proof of Theorem 9 with respect to variable y and times the result with the same variable, we will have the required result of the operator $D_y(\Pi(I''J_m(n,n); x, y))$, for the structure of Y-type junction which is $I''J_m(n,n)$.

$$
\begin{aligned}
D_y(\Pi(I''J_m(n,n);x,y)) &= y\frac{\partial \Pi(I''J_m(n,n))}{\partial y}\\
&= y\frac{\partial}{\partial y}\left((8k)xy^3 + (2k)x^2y^2 + (4k)x^2y^3 + \left(9k^2 + 15k + 36mk + 9\right)x^3y^3\right)\\
&= y\left((24k)xy^2 + (4k)x^2y + (12k)x^2y^2 + \left(27k^2 + 45k + 108mk + 27\right)x^3y^2\right)\\
&= 24kxy^3 + 4kx^2y^2 + 12kx^2y^3 + \left(27k^2 + 45k + 108mk + 27\right)x^3y^3.
\end{aligned}
\tag{58}
$$

□

Lemma 6. *Let $I''J_m(n,n)$ be a structure of Y-third type junction with $k \geq 2$, $n = 2k$, $m \geq 1$, $S_x(\Pi(I''J_m(n,n);x,y))$ and $S_y(I''\Pi(J_m(n,n);x,y))$ are the integral operators for $I''J_m(n,n)$. Then,*

$$
S_x(\Pi(I''J_m(n,n);x,y)) = 3kx^2y^2 + 6kx^2y^3 + \left(3k^2 + k + 18mk + 3\right)x^3y^3, \tag{59}
$$

$$
S_y(\Pi(I''J_m(n,n);x,y)) = 3kx^2y^2 + 4kx^2y^3 + \left(3k^2 + k + 18mk + 3\right)x^3y^3. \tag{60}
$$

Proof. In this proof, we will provide an example for the usage of integral operators. By introducing a new parameter in the place of a variable x and integrating the equation given in the proof of Theorem 9 with respect to the same variable, let say z and times the result with the same variable, we will have the required result of operator $S_x(\Pi(I''J_m(n,n);x,y))$, for the structure of Y-type junction which is $I''J_m(n,n)$.

$$
\begin{aligned}
S_x(\Pi(I''J_m(n,n);x,y)) &= \int_0^x \frac{\Pi(I''J_m(n,n);z,y)}{z}\mathrm{d}z\\
&= \int_0^x \frac{1}{z}\left((8k)zy^3 + (2k)z^2y^2 + (4k)z^2y^3 + \left(9k^2 + 15k + 36mk + 9\right)z^3y^3\right)\mathrm{d}z\\
&= \int_0^x (8k)y^3 + \int_0^x (2k)zy^2 + \int_0^x (4k)zy^3 + \int_0^x \left(9k^2 + 15k + 36mk + 9\right)z^2y^3\mathrm{d}z\\
&= (8k)zy^3|_0^x| + (2k)z^2y^2|_0^x + (4k)z^2y^3|_0^x + \left(9k^2 + 15k + 36mk + 9\right)z^3y^3|_0^x\\
&= 3kx^2y^2 + 6kx^2y^3 + \left(3k^2 + k + 18mk + 3\right)x^3y^3.
\end{aligned}
\tag{61}
$$

Similarly, by introducing a new parameter in the place of variable y and integrating the equation given in the proof of Theorem 9 with respect to the same variable, let say z and times the result with same variable, we will have the required result of operator $S_y(\Pi(I''J_m(n,n);x,y))$, for the structure of Y-type junction which is $I''J_m(n,n)$.

$$
\begin{aligned}
S_y(\Pi(I''J_m(n,n);x,y)) &= \int_0^y \frac{\Pi(J_m(n,n);x,z)}{z}\,dz\\
&= \int_0^y \frac{1}{z}\left((8k)xz^3 + (2k)x^2z^2 + (4k)x^2z^3 + \left(9k^2 + 15k + 36mk + 9\right)x^3z^3\right)dz\\
&= \int_0^y (8k)xz^2 + \int_0^y (2k)x^2z + \int_0^y (4k)x^2z^2 + \int_0^y \left(9k^2 + 15k + 36mk + 9\right)x^3z^2\,dz\\
&= (8k)xz^2 + \int_0^y (2k)x^2z + \int_0^y (4k)x^2z^2 + \int_0^y \left(9k^2 + 15k + 36mk + 9\right)x^3z^2\Big|_0^y\\
&= 3kx^2y^2 + 4kx^2y^3 + \left(3k^2 + k + 18mk + 3\right)x^3y^3.
\end{aligned}
\tag{62}
$$

□

Theorem 10. *Let $I''J_m(n,n)$ be a structure of Y-third type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $\Pi_{M_1}(I''J_m(n,n);x,y)$ is the first Zagreb M-polynomials for $I''J_m(n,n)$. Then,*

$$
\begin{aligned}
\prod_{M_1}(I''J_m(n,n)) &= 32kxy^3 + 8kx^2y^2 + 20kx^2y^3\\
&\quad + \left(54k^2 + 90k + 216mk + 54\right)x^3y^3.
\end{aligned}
\tag{63}
$$

Proof. A method to compute the first Zagreb M-polynomial is given in equation (4) of Definition 4, and this methodology is derived from the basic formula of the first Zagreb index given in equation (2) of Definition 2. Now, by using the differential operator of $I''J_m(n,n)$, defined in the Lemma 5 and applying it to the equation (4), we will have the required result of the first Zagreb M-polynomial of $I''J_m(n,n)$, which is computed as follows:

$$
\begin{aligned}
\prod_{M_1}(I''J_m(n,n)) &= \left(D_x + D_y\right)(\Pi(I''J_m(n,n)))\\
&= D_x(\Pi(I''J_m(n,n))) + D_y(\Pi(I''J_m(n,n)))\\
&= (8k)xy^3 + (4k)x^2y^2 + (8k)x^2y^3 + \left(27k^2 + 45k + 108mk + 27\right)x^3y^3\\
&\quad + (24k)xy^3 + (4k)x^2y^2 + (12k)x^2y^3 + \left(27k^2 + 45k + 108mk + 27\right)x^3y^3\\
&= 32kxy^3 + 8kx^2y^2 + 20kx^2y^3 + \left(54k^2 + 90k + 216mk + 54\right)x^3y^3.
\end{aligned}
\tag{64}
$$

□

Theorem 11. *Let $I''J_m(n,n)$ be a structure of Y-third type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $\Pi_{M_2}(I''J_m(n,n);x,y)$ is the second Zagreb M-polynomials for $I''J_m(n,n)$. Then,*

$$
\begin{aligned}
\prod_{M_2}(I''J_m(n,n)) &= 24kxy^3 + 8kx^2y^2 + 24kx^2y^3\\
&\quad + \left(81k^2 + 135k + 324mk + 81\right)x^3y^3.
\end{aligned}
\tag{65}
$$

Proof. A method to compute the second Zagreb M-polynomial is given in equation (5) of Definition 4, and this methodology is derived from the basic formula of the second Zagreb index given in equation (3) of Definition 3. Now, by using the differential operator of $I''J_m(n,n)$, defined in the Lemma 5 and applying it to equation (5), we will have the required result of the second Zagreb M-polynomial of $I''J_m(n,n)$, which is computed as follows:

$$
\begin{aligned}
\prod_{M_2}(I''J_m(n,n)) &= \left(D_xD_y\right)(\Pi(I''J_m(n,n)))\\
&= D_x\left((24k)xy^3 + (4k)x^2y^2 + (12k)x^2y^3 + \left(27k^2 + 45k + 108mk + 27\right)x^3y^3\right)\\
&= 24kxy^3 + 8kx^2y^2 + 24kx^2y^3 + \left(81k^2 + 135k + 324mk + 81\right)x^3y^3.
\end{aligned}
\tag{66}
$$

□

Theorem 12. *Let $I''J_m(n,n)$ be a structure of Y-third type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $\Pi_{R_\alpha}(I''J_m(n,n);x,y)$ is the general Randić M-polynomials for $I''J_m(n,n)$. Then,*

$$\prod_{R_\alpha}\left(I'' J_m(n,n)\right) = 3^\alpha (8k)xy^3 + 4^\alpha (2k)x^2y^2 + 6^\alpha (4k)x^2y^3 + 9^\alpha\left(9k^2 + 15k + 36mk + 9\right)x^3y^3. \tag{67}$$

Proof. A method to compute the generalized Randić M-polynomial is given in equation (7) of Definition 5, and this methodology is derived from the basic formula of the generalized Randić index given in equation (6) of Definition 5. Now, by using the generalized view of differential operators of $I'' J_m(n,n)$, defined in the Lemma 5 and applying it to equation (7), we will have the required result of generalized Randić M-polynomial of $I'' J_m(n,n)$, which is computed as follows:

$$\begin{aligned}\prod_{R_\alpha}\left(I'' J_m(n,n)\right) &= \left(D_x^\alpha D_y^\alpha\right)\left(\Pi\left(I'' J_m(n,n)\right)\right)\\ &= \left(D_x^\alpha D_y^\alpha\right)\left((8k)xy^3 + (2k)x^2y^2 + (4k)x^2y^3 + \left(9k^2 + 15k + 36mk + 9\right)x^3y^3\right)\\ &= 3^\alpha (8k)xy^3 + 4^\alpha (2k)x^2y^2 + 6^\alpha (4k)x^2y^3 + 9^\alpha\left(9k^2 + 15k + 36mk + 9\right)x^3y^3.\end{aligned} \tag{68}$$

□

5. $I''' J_m(n,n)$ Structure of Y-Fourth Type Junction

Theorem 13. *Let $I''' J_m(n,n)$ be a structure of Y-fourth type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $\Pi(I''' J_m(n,n); x, y)$ is the general M-polynomials for $I''' J_m(n,n)$. Then,*

$$\Pi\left(I''' J_m(n,n); x, y\right) = 12kxy^3 + \left(9k^2 + 21k + 36mk + 9\right)x^3y^3. \tag{69}$$

Proof. From Figure 2, which is the construction for the structure of the Y-second type junction, we can observe that there are two edge partitions based on the degree of end vertices of each edge that is defined as

$$\begin{aligned} e_{1,3} &= \left\{uv \in E\left(I''' J_m(n,n)\right): d(u) = 1,\ d(v) = 3\right\},\\ e_{3,3} &= \left\{uv \in E\left(I''' J_m(n,n)\right): d(u) = d(v) = 3\right\}.\end{aligned} \tag{70}$$

The numbers of these edge types are $|e_{1,3}| = 12k$ and $|e_{3,3}| = 9k^2 + 21k + 36mk + 9$. Then, from the Definition 1, the M-polynomial of $I''' J_m(n,n)$ can be found as

$$\begin{aligned}\Pi\left(I'' \prime\prime J_m(n,n); x, y\right) &= \sum_{i \leq j} m_{i,j}\left(I'' \prime\prime J_m(n,n)\right)x^i y^j\\ &= 12kxy^3 + \left(9k^2 + 21k + 36mk + 9\right)x^3y^3.\end{aligned} \tag{71}$$

□

Lemma 7. *Let $I''' J_m(n,n)$ be a structure of Y-fourth type junction with $k \geq 2$, $n = 2k$, $m \geq 1$, $D_x(\Pi(I''' J_m(n,n); x, y))$ and $D_y(I'''\Pi(J_m(n,n); x, y))$ are the integral operators for $I''' J_m(n,n)$. Then,*

$$D_x\left(\Pi\left(I''' J_m(n,n); x, y\right)\right) = 12kxy^3 + \left(27k^2 + 63k + 108mk + 27\right)x^3y^3, \tag{72}$$

$$D_y\left(\Pi\left(I''' J_m(n,n); x, y\right)\right) = 36kxy^3 + \left(27k^2 + 63k + 108mk + 27\right)x^3y^3. \tag{73}$$

Proof. In this proof, we will provide an example for the usage of differential operators. By differentiating the equation given in the proof of Theorem 13 with respect to variable x and times the result with the same variable, we will have the required result of the operator $D_x(\Pi\ (I''' J_m(n,n); x, y))$, for the structure of Y-type junction which is $I''' J_m(n,n)$.

$$\begin{aligned} D_x\left(\Pi\left(I'''J_m(n,n);x,y\right)\right) &= x\frac{\partial\Pi\left(I'''J_m(n,n)\right)}{\partial x}\\ &= x\frac{\partial}{\partial x}\left((12k)xy^3+\left(9k^2+21k+36mk+9\right)x^3y^3\right)\\ &= x\left((12k)y^3+\left(27k^2+63k+108mk+27\right)x^2y^3\right)\\ &= 12kxy^3+\left(27k^2+63k+108mk+27\right)x^3y^3. \end{aligned} \tag{74}$$

Similarly, by differentiating the equation given in the proof of Theorem 13 with respect to variable y and times the result with the same variable, we will have the required result of the operator $D_y(\Pi(I'''J_m(n,n);x,y))$, for the structure of Y-type junction which is $I'''J_m(n,n)$.

$$\begin{aligned} D_y\left(\Pi\left(I'''J_m(n,n);x,y\right)\right) &= y\frac{\partial\Pi\left(I'''J_m(n,n)\right)}{\partial y}\\ &= y\frac{\partial}{\partial x}\left((12k)xy^3+\left(9k^2+21k+36mk+9\right)x^3y^2\right)\\ &= y\left((36k)xy^2+\left(27k^2+63k+108mk+27\right)x^3y^2\right)\\ &= 36kxy^3+\left(27k^2+63k+108mk+27\right)x^3y^3. \end{aligned} \tag{75}$$

□

Lemma 8. *Let $I'''J_m(n,n)$ be a structure of Y-fourth type junction with $k\geq 2$, $n=2k$, $m\geq 1$, $S_x(\Pi(I'''J_m(n,n);x,y))$ and $S_y(I'''\Pi(J_m(n,n);x,y))$ are the integral operators for $I'''J_m(n,n)$. Then,*

$$S_x\left(\Pi\left(I'''J_m(n,n);x,y\right)\right) = 3kx^2y^2+6kx^2y^3+\left(3k^2+k+18mk+3\right)x^3y^3, \tag{76}$$

$$S_y = 3kx^2y^2+4kx^2y^3+\left(3k^2+k+18mk+3\right)x^3y^3. \tag{77}$$

Proof. In this proof, we will provide an example for the usage of integral operators. By introducing a new parameter in the place of variable x and integrating the equation given in the proof of Theorem 13 with respect to the same variable, let say z and times the result with the same variable, we will have the required result of the operator $S_x(\Pi(I'''J_m(n,n);x,y))$, for the structure of Y-type junction which is $I'''J_m(n,n)$.

$$\begin{aligned} S_x\left(\Pi\left(I'''J_m(n,n);x,y\right)\right) &= \int_0^x\frac{\Pi\left(I'''J_m(n,n);z,y\right)}{z}\mathrm{d}z\\ &= \int_0^x\frac{1}{z}\left(12kzy^3+\left(9k^2+21k+36mk+9\right)z^3y^3\right)\mathrm{d}z\\ &= \int_0^x(12k)y^3+\int_0^x\left(9k^2+21k+36mk+9\right)z^2y^3z\\ &= (12k)zy^3\big|_0^x+\left(9k^2+21k+36mk+9\right)z^3y^3\big|_0^x\\ &= 3kx^2y^2+6kx^2y^3+\left(3k^2+k+18mk+3\right)x^3y^3. \end{aligned} \tag{78}$$

Similarly, by introducing a new parameter in the place of variable y, and integrating the equation given in the proof of Theorem 13 with respect to the same variable, let say z and times the result with the same variable, we will have the required result of the operator $S_y(\Pi(I'''J_m(n,n);x,y))$, for the structure of Y-type junction which is $I'''J_m(n,n)$.

$$
\begin{aligned}
S_y\left(\Pi\left(I''' J_m(n,n); x, y\right)\right) &= \int_0^x \frac{\Pi\left(I''' J_m(n,n); x, z\right)}{z} \mathrm{d}z \\
&= \int_0^y \frac{1}{z}\left((12k)xz^3 + \left(9k^2 + 21k + 36mk + 9\right)x^3z^3\right)\mathrm{d}z \\
&= \int_0^y (12k)xz^2 dz + \int_0^y \left(9k^2 + 21k + 36mk + 9\right)x^3z^2z\mathrm{d}z \\
&= (12k)x\frac{z^3}{3}\Big|_0^y + \left(9k^2 + 21k + 36mk + 9\right)x^3\frac{z^3}{3}\Big|_0^y \\
&= 3kx^2y^2 + 4kx^2y^3 + \left(3k^2 + k + 18mk + 3\right)x^3y^3.
\end{aligned} \tag{79}
$$

□

Theorem 14. *Let $I''' J_m(n,n)$ be a structure of Y-fourth type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $\Pi_{M_1}(I''' J_m(n,n); x, y)$ is the first Zagreb M-polynomials for $I''' J_m(n,n)$. Then,*

$$
\begin{aligned}
\prod_{M_1}\left(I''' J_m(n,n)\right) &= 48kxy^3 \\
&\quad + \left(54k^2 + 126k + 216mk + 54\right)x^3y^3.
\end{aligned} \tag{80}
$$

Proof. A method to compute the first Zagreb M-polynomial is given in equation (4) of Definition 4, and this methodology is derived from the basic formula of the first Zagreb index given in equation (2) of Definition 2. Now, by using the differential operator of $I''' J_m(n,n)$, defined in the Lemma 7 and applying it to Equation 4, we will have the required result of the first Zagreb M-polynomial of $I''' J_m(n,n)$, which is computed as follows:

$$
\begin{aligned}
\prod_{M_1}\left(I''' J_m(n,n)\right) &= \left(D_x + D_y\right)\left(\Pi\left(I''' J_m(n,n)\right)\right) \\
&= D_x\left(\Pi\left(I''' J_m(n,n)\right)\right) + D_y\left(\Pi\left(I''' J_m(n,n)\right)\right) \\
&= (12k)xy^3 + \left(27k^2 + 63k + 108mk + 27\right)x^3y^3 + (36k)xy^3 + \left(27k^2 + 63k + 108mk + 27\right)x^3y^3 \\
&= 48kxy^3 + \left(54k^2 + 126k + 216mk + 54\right)x^3y^3.
\end{aligned} \tag{81}
$$

□

Theorem 15. *Let $I''' J_m(n,n)$ be a structure of Y-fourth type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $\Pi_{M_2}(I''' J_m(n,n); x, y)$ is the second Zagreb M-polynomials for $I''' J_m(n,n)$. Then,*

$$
\begin{aligned}
\prod_{M_2}\left(I''' J_m(n,n)\right) &= 36kxy^3 \\
&\quad + \left(81k^2 + 189k + 324mk + 27\right)x^3y^3.
\end{aligned} \tag{82}
$$

Proof. A method to compute the second Zagreb M-polynomial is given in equation (5) of Definition 4, and this methodology is derived from the basic formula of the second Zagreb index given in equation (3) of Definition 3. Now, by using the differential operator of $I''' J_m(n,n)$, defined in the Lemma 7 and applying it to equation (5), we will have the required result of the second Zagreb M-polynomial of $I''' J_m(n,n)$, which is computed as follows:

$$
\begin{aligned}
\prod_{M_2}\left(I''' J_m(n,n)\right) &= \left(D_xD_y\right)\left(\Pi\left(I''' J_m(n,n)\right)\right) \\
&= D_x\left((36k)xy^3 + \left(27k^2 + 63k + 108mk + 9\right)x^3y^3\right) \\
&= 36kxy^3 + \left(81k^2 + 189k + 324mk + 27\right)x^3y^3.
\end{aligned} \tag{83}
$$

□

Theorem 16. *Let $I''' J_m(n,n)$ be a structure of Y-fourth type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $\Pi_{R_\alpha}(I''' J_m(n,n); x, y)$ is the general Randić M-polynomials for $I''' J_m(n,n)$. Then,*

$$\prod_{R_\alpha}\left(I''' J_m(n,n)\right) = 3^\alpha (12k)xy^3 + 3^{2\alpha}\left(9k^2 + 21k + 36mk + 9\right)x^3y^3. \tag{84}$$

Proof. A method to compute the generalized Randić M-polynomial is given in equation (7) of Definition 1, and this methodology is derived from the basic formula of the generalized Randić index given in equation (6) of Definition 5. Now, by using the generalized view of differential operators of $I''' J_m(n,n)$, defined in the Lemma 7, and applying it to equation (7), we will have the required result of generalized Randić M-polynomial of $I''' J_m(n,n)$, which is computed as follows:

$$\begin{aligned}\prod_{R_\alpha}\left(I''' J_m(n,n)\right) &= \left(D_x^\alpha D_y^\alpha\right)\left(\Pi\left(I''' J_m(n,n)\right)\right)\\ &= \left(D_x^\alpha D_y^\alpha\right)\left(12kxy^3 + \left(9k^2 + 21k + 36mk + 9\right)x^3y^3\right)\\ &= 3^\alpha (12k)xy^3 + 3^{2\alpha}\left(9k^2 + 21k + 36mk + 9\right)x^3y^3.\end{aligned} \tag{85}$$

□

6. Verifications of Topological Indices

There are some techniques to find the authenticity or correctness of topological indices. M-polynomial is one of the techniques. By using Theorems 2 to 4, we can verify the main results of topological indices given in the [36], for the structure of Y-type junction or $J_m(n,n)$. Similarly, for the results of the structure of Y-second type junction or $I' J_m(n,n)$, we can use the results of our main Theorems 6 to 8 and use the values of $x = y = 1$. For the results of the structure of the Y-third type junction or $I'' J_m(n,n)$, we can use the results of our main Theorems 10 to 12 while Theorems 14 to 16 are used to verify the results of the structure of the Y-fourth type junction or $I''' J_m(n,n)$, given as follows.

Theorem 17. *Let $J_m(n,n)$ be a structure of Y-type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $M_1(J_m(n,n))$ is the first Zagreb index for $J_m(n,n)$. Then,*

$$M_1(J_m(n,n)) = 102k + 54k^2 + 216mk + 54. \tag{86}$$

Theorem 18. *Let $J_m(n,n)$ be a structure of Y-type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $M_2(J_m(n,n))$ is the second Zagreb index for $J_m(n,n)$. Then,*

$$M_2(J_m(n,n)) = 123k + 81k^2 + 324mk + 81. \tag{87}$$

Theorem 19. *Let $J_m(n,n)$ be a structure of Y-type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $R_\alpha(J_m(n,n))$ is the general Randić index for $J_m(n,n)$. Then,*

$$R_\alpha(J_m(n,n)) = 4^\alpha (6k) + 6^\alpha (12k) + 9^\alpha\left(9k^2 + 3k + 36mk + 9\right). \tag{88}$$

Theorem 20. *Let $J_m(n,n)$ be a structure of Y-second type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $M_1(I' J_m(n,n))$ is the first Zagreb index for $I' J_m(n,n)$. Then,*

$$M_1(I' J_m(n,n)) = 126k + 54k^2 + 216mk + 54. \tag{89}$$

Theorem 21. *Let $J_m(n,n)$ be a structure of Y-second type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $M_2(I' J_m(n,n))$ is the second Zagreb index for $I' J_m(n,n)$. Then,*

$$M_2(I' J_m(n,n)) = 157k + 81k^2 + 324mk + 81. \tag{90}$$

Theorem 22. *Let $J_m(n,n)$ be a structure of Y-second type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $R_\alpha(I' J_m(n,n))$ is the general Randić index for $I' J_m(n,n)$. Then,*

$$R_\alpha(I' J_m(n,n)) = 3^\alpha (4k) + 2^{2\alpha} (4k) + 6^\alpha (8k) + 3^{2\alpha}\left(9k^2 + 9k + 36mk + 9\right). \tag{91}$$

Theorem 23. *Let $I'' J_m(n,n)$ be a structure of Y-third type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $M_1(I'' J_m(n,n))$ is the first Zagreb index for $I'' J_m(n,n)$. Then,*

$$M_1(I'' J_m(n,n)) = 150k + 54k^2 + 216mk + 54. \tag{92}$$

Theorem 24. *Let $I'' J_m(n,n)$ be a structure of Y-third type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $M_2(I'' J_m(n,n))$ is the second Zagreb index for $I'' J_m(n,n)$. Then,*

$$M_2(I'' J_m(n,n)) = 191k + 81k^2 + 324mk + 81. \tag{93}$$

Theorem 25. *Let $I'' J_m(n,n)$ be a structure of Y-third type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $R_\alpha(I'' J_m(n,n))$ is the general Randić index for $I'' J_m(n,n)$. Then,*

$$R_\alpha(I'' J_m(n,n)) = 3^\alpha (8k) + 4^\alpha (2k) + 6^\alpha (4k) + 9^\alpha\left(9k^2 + 15k + 36mk + 9\right). \tag{94}$$

Theorem 26. *Let $I''' J_m(n,n)$ be a structure of Y-fourth type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $M_1(I''' J_m(n,n))$ is the first Zagreb index for $I''' J_m(n,n)$. Then,*

$$M_1\left(I''' J_m(n,n)\right) = 174k + 54k^2 + 216mk + 54. \quad (95)$$

Theorem 27. *Let $I''' J_m(n,n)$ be a structure of Y-fourth type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $M_2(I''' J_m(n,n))$ is the second Zagreb index for $I''' J_m(n,n)$. Then,*

$$M_2\left(I''' J_m(n,n)\right) = 225k + 81k^2 + 324mk + 81. \quad (96)$$

Theorem 28. *Let $I''' J_m(n,n)$ be a structure of Y-fourth type junction with $k \geq 2$, $n = 2k$, $m \geq 1$ and $R_\alpha(I''' J_m(n,n))$ is the general Randić index for $I''' J_m(n,n)$. Then,*

$$R_\alpha\left(I''' J_m(n,n)\right) = 3^\alpha(12k) + 3^{2\alpha}\left(9k^2 + 15k + 36mk + 9\right). \quad (97)$$

From the above discussion, the topological indices, given in the [36], are found correct, and calculations are verified here with M-polynomials methodology.

7. Conclusion

In this research work, vertex-degree-based M-polynomials of Y-junctions and their variants are studied for the first time. We determined general Randić first and second Zagreb vertex-degree-based M-polynomials for four types of Y-shaped carbon nanotube junctions $J_m(n,n)$. By this method, Y-junctions and their structures are elaborated in numerical form, and the whole compound is described as a numeric digit. Instead of a whole complex structure, it will be easy to see as a numeric quantity. Furthermore, we verified the results from literature given on the concept of the topological index from the method of vertex-degree-based M-polynomials and concluded that the results are calculated correctly in the literature.

Data Availability

All data used to support the study are included within the manuscript.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

M. K. Jamil conceived the presented idea. Aisha Javed developed the theory and performed the computations. M. Azeem verified and investigated the analytical methods, and Ali Ahmad supervised the findings of this work. All authors discussed the results and contributed to the final manuscript.

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