Research Article

Comparative Study of Y-Junction Nanotubes with Vertex-Edge Based Topological Descriptors

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The current results of various forms of carbon nanostructures and its applications in different areas attract the researchers. In pharmaceutical, medicine, industry and electronic devices they used it by its graphical invariants. The detection of different types of carbon nanotubes junctions enhanced the attention and interest for forthcoming devices like transistors and amplifiers. A topological index plays a very important role in the study of physicochemical properties of biological and chemical structures. In this paper, we determine results of \( \text{ve} \)-degree topological indices for various type of carbon nanotubes Y-junctions and their comparisons. The particular indices called as The first \( \text{ve} \)-degree Zagreb \( \beta \) index, the second \( \text{ve} \)-degree Zagreb index, \( \text{ve} \)-degree Randic index, \( \text{ve} \)-degree atom-bond connectivity index, \( \text{ve} \)-degree geometric-arithmetic index, \( \text{ve} \)-degree harmonic index and \( \text{ve} \)-degree sum-connectivity index.

1. Introduction

Let a graph having vertex set \( V \) and edge set \( E \) possesses the properties of connectivity, usually labeled as \( G = (V, E) \). For a vertex \( x_1 \in V \), the concept of open neighborhood of that vertex \( x_1 \) is formulated as \( N(x_1) = \{x_2 \in V: x_1x_2 \in E\} \), while the concept of closed neighborhood formulated and notated by \( N[x_1] = N(x_1) \cup x_1 \). A notation \( \xi_{ve}(x_1) \), is used for the \( \text{ve} \)-degree of any vertex \( x_1 \in V \), and measured by the count of distinct edges which are incident to any vertex from the closed neighborhood of \( x_1 \). Further detail and discussion on this notation and its mathematical definition, one can see [4–6].

In molecular graph theory, vertices and edges are replaced by atoms and their bonds while transforming from a molecular structure to a molecular graph, respectively, [7, 8]. Carbon nanotubes with branching ends are promising building blocks for next-generation enhanced nanoelectronics and nanodevices. In the junction family, three-terminal devices and carbon nanotube graphs have tremendous potential. While study the chemical things for various determinations in different areas, the energy bond is the one of the most important thermophysical to be measured. There are different type of nanotubes junctions for example, \( X, Y, L \) and \( T \) and their applications can be seen in [9–12].

The topological descriptor of a given graph is a numeric number that describes the quantitative structural-property relationship and quantitative structural-activity of the molecular graph [13–16]. The researcher in [17] discussed the metal-organic network, supramolecular chain is discussed by [18], carbon nanotubes are measured in [19] with different parameters of graph-based chemical theory. For study of different types of topological indices, see [20–25]. Some new variants and generalized results on the topological descriptors are found in the articles suggested [3, 26, 27].

There are variety of topological descriptors, one of them is the vertex-edge based that will be discussed in this article. The researchers in [1], defined the “\( \text{ve} \)-degree,” and [4] contributed in this study. Basic definitions regarding “\( \text{ve} \)-degree” topological indices, refer to [28].

The vertex-edge based topological descriptors are: The first \( \text{ve} \)-degree Zagreb \( \beta \) index \( M_{\text{ve}}^1(Y_{mn}(n,n)) = \Sigma_{x_1x_2 \in E} (\xi_{ve}(x_1) + \xi_{ve}(x_2)) \), the second \( \text{ve} \)-degree Zagreb index
\( (M^2_{ve}(Y_m(n,n)) = \sum_{x_i, x_j \in E} (\xi_{ve}(x_1) \times \xi_{ve}(x_2)), \) ve-degree Randić index \((R_{ve}(Y_m(n,n)) = \sum_{x_i, x_j \in E} (\xi_{ve}(x_1) \times \xi_{ve}(x_2))^{1/2}), \) ve-degree atom-bond connectivity index \((ABC_{ve}(Y_m(n,n)) = \sum_{x_i, x_j \in E} ((\xi_{ve}(x_1) + \xi_{ve}(x_2) - 2)/ (\xi_{ve}(x_1) \times \xi_{ve}(x_2)))^{1/2}), \) ve-degree geometric-arithmetic index \((GA_{ve}(Y_m(n,n)) = \sum_{x_i, x_j \in E} (2(\xi_{ve}(x_1) \times \xi_{ve}(x_2)))^{1/2})), \) ve-degree harmonic index \((H_{ve}(Y_m(n,n)) = \sum_{x_i, x_j \in E} (2(\xi_{ve}(x_1) + \xi_{ve}(x_2)))) \) and ve-degree sum-connectivity index \((\chi_{ve}(Y_m(n,n)) = \sum_{x_i, x_j \in E} (\xi_{ve}(x_1) + \xi_{ve}(x_2))^{1/2})). \) For further results and detail on vertex-edge based topological indices see [29, 30]. Some other related topics based on the information of edges of a graph are detailed in [31–37]. In this paper, the exact values of vertex-edge based topological indices for Y-junctions carbon nanotubes are determined.

2. Y-Junction Graphs

The Y-junctions investigated in this paper are formed by the covalent interconnection of three finite-length armchair single-walled nanotubes that intersect at a 120° angle and are specified by the chiral vector \((n,n)\). For detail study of structures, authors refer to [38–41]. A Y-junction graph is defined as follows:

Let \( n \) is even and \( m,n \) are two integers. A graph of Y-junction labeled as \( Y_m(n,n) \) is constructed by using an armchair \( Y(n,n) \), and three CNTs \( T_m \) single-walled armchair which are identical having \( m \) hexagons-layers. Total face count is \( (3n^2/4) - (3n/2) + 5 \) and hexagons count is six, hexagons count is \( (3n^2/4) - (3n/2) - 5 \). Furthermore, each armchair tube labeled by \( T_m \) contained hexagonal-faces of count \( 2mn \). The degree two count vertices are \( 6n \), degree three three with count \( (3n^2/2) + 3n + 12mn + 6 \), collectively having \( (3n^2/2) + 9n + 12mn + 6 \) order, and \( (9n^2/4) + (21n/2) + 18mn + 9 \) size.

In this work, a junction graph labeled with \( Y_m(n,n) \) is graphs having no pendant or degree one vertex, exists. This work also consists of other three topologies of Y-junction graphs labeled with \( Y^1_m(n,n), Y^2_m(n,n) \) and \( Y^3_m(n,n) \) and these contained some vertices with degree one. These further topologies are constructed by \( Y_m(n,n) \)-junction graphs by adding pendants to degree 2 vertices. Single tube among three tubes of \( Y_m(n,n) \) has exactly \( 2n \) count of vertices having two degree. In result, \( 6n \) is the maximum number of pendants that can be utilised with this attachment for \( Y_m(n,n) \) and \( 2n \) for each tube.

3. The ve-Degree Results of Y-Junction Graph \( Y_m(n,n) \)

This section presented the ve-degree results of Y-junction graph \( Y_m(n,n) \). This graph does not contain any pendant vertex that is shown in Figure 1. The edge partition of end vertices ve-degree of each edge along with the degree of end vertices of each edge for \( Y_m(n,n) \) graph is given in Table 1.

| (\(\xi_{ve}(x_1), \xi_{ve}(x_2)\)) | \(\xi_{ve}(x_1)\times\xi_{ve}(x_2)\) | Count |
|-------------------------------|-----------------------------------|-------|
| (2,2)        | (5,5)                             | 3n    |
| (2,3)        | (5,8)                             | 6n    |
| (3,3)        | (8,9)                             | 6n    |
| (3,3)        | (9,9)                             | \((9n^2/4) - (9n/2) + 18mn + 9\) |

3.1. The First ve-Degree Zagreb β Index.

\[ M^2_{β_{ve}}(Y_m(n,n)) = \sum_{x_i, x_j \in E} (\xi_{ve}(x_1) + \xi_{ve}(x_2)) \]

\[ = (10)(3n) + (13)(6n) + (17)(6n) + (18)\left(\frac{9n^2}{4} - \frac{9n}{2} + 18mn + 9\right) \]

= \(81n^2/2 + 129n + 324mn + 162\).

3.2. The Second ve-Degree Zagreb Index.

\[ M^2_{ω_{ve}}(Y_m(n,n)) = \sum_{x_i, x_j \in E} (\xi_{ve}(x_1) \times \xi_{ve}(x_2)) \]

\[ = (25)(3n) + (40)(6n) + (72)(6n) + (81)\left(\frac{9n^2}{4} - \frac{9n}{2} + 18mn + 9\right) \]

= \(729n^2/2 + 765n + 1458mn + 729\).

3.3. The Randić Index Developed by ve-Degree Methodology.

Utilizing the edge-partition details described in the Table 1, we measured the Randić index developed by ve-degree methodology:
\[
R_{\text{ve}}(Y_m(n,n)) = \sum_{x_i,x_j \in E} \left( \frac{\xi_{\text{ve}}(x_1) \times \xi_{\text{ve}}(x_2)}{\xi_{\text{ve}}(x_1) \times \xi_{\text{ve}}(x_2)} \right)^{-1/2}
\]

\[
= (25)^{-1/2} (3n) + (40)^{-1/2} (6n) + (72)^{-1/2} (6n) + (81)^{-1/2} \left( \frac{9n^2}{4} - \frac{9n}{2} + 18mn + 9 \right)
\]

\[
= n^2 \left( \frac{1}{4} + \frac{3\sqrt{10}}{10} + \frac{\sqrt{2}}{2} + 2m \right) n + 1.
\]

3.4. The Atom-Bond Connectivity Index Developed by ve-Degree Methodology. Utilizing the edge-partition details described in the Table 1, we measured the atom-bond connectivity index developed by ve-degree methodology:

\[
ABC_{\text{ve}}(Y_m(n,n)) = \sum_{x_i,x_j \in E} \left( \frac{\xi_{\text{ve}}(x_1) + \xi_{\text{ve}}(x_2) - 2}{\xi_{\text{ve}}(x_1) \times \xi_{\text{ve}}(x_2)} \right)^{-1/2}
\]

\[
= (3n) \left( \frac{8}{25} + \frac{6n}{10} \right) + (6n) \left( \frac{15}{72} + \left( \frac{9n^2}{4} - \frac{9n}{2} + 18mn + 9 \right) \right)
\]

\[
= n^2 + \left( \frac{6\sqrt{2}}{5} + \frac{3\sqrt{10}}{10} + \frac{\sqrt{30}}{2} + 8m - 2 \right) n + 4.
\]

3.5. The Geometric-Arithmetic Index Developed by ve-Degree Methodology. Utilizing the edge-partition details described in the Table 1, we measured the geometric-arithmetic index developed by ve-degree methodology:

\[
GA_{\text{ve}}(Y_m(n,n)) = \sum_{x_i,x_j \in E} \left( \frac{2(\xi_{\text{ve}}(x_1) \times \xi_{\text{ve}}(x_2))^{1/2}}{\xi_{\text{ve}}(x_1) + \xi_{\text{ve}}(x_2)} \right)
\]

\[
= (3n) \left( \frac{2\sqrt{25}}{10} + \frac{6n}{13} \right) \left( \frac{2\sqrt{40}}{17} + \frac{6n}{17} \right) \left( \frac{9n^2}{4} - \frac{9n}{2} + 18mn + 9 \right)
\]

\[
= \frac{9n^2}{4} + \left( \frac{-3}{2} + \frac{24\sqrt{10}}{13} + \frac{72\sqrt{2}}{17} + 18m \right) n + 9.
\]

3.6. The Harmonic Index Developed by ve-Degree Methodology. Utilizing the edge-partition details described in the Table 1, we measured the harmonic index developed by ve-degree methodology:

\[
H_{\text{ve}}(Y_m(n,n)) = \sum_{x_i,x_j \in E} \left( \frac{2}{\xi_{\text{ve}}(x_1) + \xi_{\text{ve}}(x_2)} \right)
\]

\[
= (3n) \left( \frac{2}{10} + \frac{6n}{13} \right) \left( \frac{2}{17} + \left( \frac{9n^2}{4} - \frac{9n}{2} + 18mn + 9 \right) \right)
\]

\[
= n^2 + \left( \frac{3821}{2210} + 2m \right) n + 1.
\]
3.7. The Sum-Connectivity Index Developed by ve-Degree Methodology. Utilizing the edge-partition details described in the Table 1, we measured the sum-connectivity index developed by ve-degree methodology:

\[
\chi \text{ve}(Y_m(n,n)) = \sum_{x_i,x_j \in E} (\xi \text{ve}(x_i) + \xi \text{ve}(x_j))^{(-1/2)} \\
= (3n) \left( \frac{1}{\sqrt{10}} + (6n) \frac{1}{\sqrt{13}} + (6n) \frac{1}{\sqrt{17}} + \left( \frac{9n^2}{4} - \frac{9n}{2} + 18mn + 9 \right) \right) \frac{1}{\sqrt{18}} \\
= \frac{3\sqrt{2}n^2}{8} + \left( \frac{3\sqrt{10}}{10} + \frac{6\sqrt{13}}{13} + \frac{6\sqrt{17}}{17} + \frac{\sqrt{2}}{6} \left( -\frac{9}{2} + 18m \right) \right) n + \frac{3\sqrt{2}}{2}.
\]

(7)

4. The ve-Degree Results of Y-Junction Graph \(Y^1_m(n,n)\)

By attaching the 2p pendants vertices with 2 degree vertices to any one tube of \(Y_m(n,n)\) graph, we obtain a new graph, it is denoted by \(Y^1_m(n,n)\), see Figure 2. The order and size of \(Y^1_m(n,n)\) graph is \((3n^2)/2 + 11n + 12mn + 6\) and \((9n^2)/4 + (25n)/2 + 18mn + 9\), respectively. This section determinen the ve-degree results of Y-junction graph \(Y^1_m(n,n)\). The edge partition of end vertices ve-degree of each edge along with the degree of end vertices of each edge for \(Y^1_m(n,n)\) graph is given in Table 2.

4.1. The First ve-Degree Zagreb \(\beta\) Index.

\[
M^1_{\text{ve}}(Y^1_m(n,n)) = \sum_{x_i,x_j \in E} (\xi \text{ve}(x_i)) \\
= (10)(2n) + (13)(4n) + (16)(2n) + (10)(2n) + (17)(4n) + (14)(n) + (18) + \left( \frac{9n^2}{4} - \frac{5n}{2} + 18mn + 9 \right) \frac{1}{2} \\
= \frac{81n^2}{2} + (161 + 324m)n + 162.
\]

(8)

4.2. The Second ve-Degree Zagreb Index.

\[
M^2_{\text{ve}}(Y^1_m(n,n)) = \sum_{x_i,x_j \in E} (\xi \text{ve}(x_i) \times \xi \text{ve}(x_j)), \\
M^2_{\text{ve}}(Y^1_m(n,n)) = (25)(2n) + (40)(4n) + (63)(2n) + (21)(2n) + (72)(4n) + (49)(n) + (81) + \left( \frac{9n^2}{4} - \frac{5n}{2} + 18mn + 9 \right) \frac{1}{2} \\
= 729 + \frac{729n^2}{4} + \left( \frac{1025}{2} + 1458m \right) n.
\]

(9)

4.3. The Randić Index Developed by ve-Degree Methodology.

Utilizing the edge-partition details described in the Table 2, we measured the Randić index developed by ve-degree methodology:
Rve Y (n, n) = \( m \binom{n}{2} + \frac{\sqrt{167}}{5} \binom{n}{3} + \frac{2\sqrt{21}}{21} \binom{n}{4} + \frac{\sqrt{2}}{3} \binom{n}{5} + n \)

4.4. The Atom-Bond Connectivity Index Developed by ve-Degree Methodology. Utilizing the edge-partition details described in the Table 2, we measured the atom-bond connectivity index developed by ve-degree methodology:

\[
R_{ve}(Y^1_m(n, n)) = \sum_{x_1, x_2 \in \mathcal{E}} (\xi_{ve}(x_1) \times \xi_{ve}(x_2))^{(-1/2)}
\]

\[
= (35)^{(-1/2)}(2n) + (40)^{(-1/2)}(4n) + (63)^{(-1/2)}(2n) + (21)^{(-1/2)}(2n)
\]

\[
+ (72)^{(-1/2)}(4n) + (49)^{(-1/2)}(n) + (81)^{(-1/2)}\left(\frac{9n^2}{4} - \frac{5n}{2} + 18mn + 9\right)
\]

\[
= 1 + \frac{n^2}{4} + \left(\frac{167}{630} + \frac{\sqrt{10}}{5} + \frac{2\sqrt{7}}{21} + \frac{2\sqrt{21}}{21} + \frac{\sqrt{2}}{3} + n\right)
\]
\[
\begin{align*}
\text{ABC}_{ve}(Y_{mn}^1(n,n)) &= \sum_{x_1,x_2 \in E} \left( \frac{\xi_{ve}(x_1) + \xi_{ve}(x_2) - 2}{\xi_{ve}(x_1) \times \xi_{ve}(x_2)} \right)^{(1/2)} \\
&= (2n) \left( \frac{8}{25} + (4n) \frac{11}{40} + (2n) \frac{14}{63} + (4n) \frac{8}{21} + (2n) \frac{15}{72} + (n) \frac{12}{49} + \frac{16}{81} \sqrt{\frac{9n^2}{4} - \frac{5n}{2} + 18mn + 9} \right) \\
&= 4 + n^2 + \left( \frac{22\sqrt{2}}{15} + \frac{\sqrt{110}}{5} + \frac{4\sqrt{42}}{21} + \frac{\sqrt{30}}{3} + \frac{2\sqrt{3}}{7} - 10 + 8m \right) n. 
\end{align*}
\]

### 4.5. The Geometric-Arithmetic Index Developed by ve-Degree Methodology

Utilizing the edge-partition details described in the Table 2, we measured the geometric-arithmetic index developed by ve-degree methodology:

\[
\begin{align*}
\text{GA}_{ve}(Y_{mn}^1(n,n)) &= \sum_{x_1,x_2 \in E} \frac{2\left(\xi_{ve}(x_1) \times \xi_{ve}(x_2)\right)^{(1/2)}}{\xi_{ve}(x_1) + \xi_{ve}(x_2)} \\
&= (2n) \left( \frac{2}{\sqrt{10}} + (4n) \frac{2}{\sqrt{13}} + (2n) \frac{2}{\sqrt{16}} + (4n) \frac{2}{\sqrt{17}} + (n) \frac{2}{\sqrt{14}} + \frac{2}{\sqrt{15}} \sqrt{\frac{9n^2}{4} - \frac{5n}{2} + 18mn + 9} \right) \\
&= 9 + n^2 \frac{9}{4} + \left( \frac{1}{2} + \frac{16\sqrt{10}}{13} + \frac{3\sqrt{7}}{4} + \frac{2\sqrt{21}}{5} + \frac{48\sqrt{5}}{17} + 18m \right) n. 
\end{align*}
\]

### 4.6. The Harmonic Index Developed by ve-Degree Methodology

Utilizing the edge-partition details described in the Table 2, we measured the harmonic index developed by ve-degree methodology:

\[
\begin{align*}
\text{H}_{ve}(Y_{mn}^1(n,n)) &= \sum_{x_1,x_2 \in E} \frac{2}{\xi_{ve}(x_1) + \xi_{ve}(x_2)} \\
&= (2n) \frac{2}{\sqrt{10}} + (4n) \frac{2}{\sqrt{13}} + (2n) \frac{2}{\sqrt{16}} + (4n) \frac{2}{\sqrt{17}} + (n) \frac{2}{\sqrt{14}} + \frac{2}{\sqrt{15}} \sqrt{\frac{9n^2}{4} - \frac{5n}{2} + 18mn + 9} \\
&= 1 + n^2 \frac{557213}{278460} + 2m n. 
\end{align*}
\]

### 4.7. The Sum-Connectivity Index Developed by ve-Degree Methodology

Utilizing the edge-partition details described in the Table 2, we measured the sum-connectivity index developed by ve-degree methodology:

\[
\begin{align*}
\chi_{ve}(Y_{mn}^1(n,n)) &= \sum_{x_1,x_2 \in E} \left( \xi_{ve}(x_1) + \xi_{ve}(x_2) \right)^{(-1/2)} \\
&= (2n) \frac{1}{\sqrt{10}} + (4n) \frac{1}{\sqrt{13}} + (2n) \frac{1}{\sqrt{16}} + (4n) \frac{1}{\sqrt{17}} + (n) \frac{1}{\sqrt{14}} + \frac{1}{\sqrt{18}} \sqrt{\frac{9n^2}{4} - \frac{5n}{2} + 18mn + 9} \\
&= \left( \frac{2\sqrt{10}}{5} + \frac{4\sqrt{13}}{13} + \frac{1}{2} + \frac{4\sqrt{17}}{17} + \frac{\sqrt{14}}{14} + \frac{\sqrt{2}}{6} \left(-\frac{5}{2} + 18m\right) \right) n + \frac{3\sqrt{2}n^2}{8} + \frac{3\sqrt{2}}{2}. 
\end{align*}
\]
5. The ve-Degree Results of Y-Junction Graph $Y^2_m(n, n)$

By attaching the $4n$ pendants vertices with 2 degree vertices to any two tube of $Y_m(n, n)$ graph, we obtain a new graph, it is denoted by $Y^2_m(n, n)$, see Figure 3. The cardinality of $Y^2_m(n, n)$ is $(3n^2/2) + 13n + 12mn + 6$ and size is $(9n^2/4) + (29n/2) + 18mn + 9$. This section determined the ve-degree results of $Y$-junction graph $Y^2_m(n, n)$. The edge partition of end vertices ve-degree of each edge along with the degree of end vertices of each edge for $Y^2_m(n, n)$ graph is given in Table 3.

5.1. The First ve-Degree Zagreb β Index.

$$M^1_{ve}(Y^2_m(n, n)) = \sum_{x_1, x_2 \in E} (\xi_{ve}(x_1) + \xi_{ve}(x_2))$$

$$= (10)(n) + (13)(2n) + (16)(4n) + (10)(4n) + (17)(2n) + (14)(2n) + (18)\left(\frac{9n^2}{4} - \frac{n}{2} + 18mn + 9\right)$$

$$= 162 + \frac{81n^2}{2} + (193 + 324m)n.$$  (15)

5.2. The Second Zagreb Index Developed by ve-Degree Methodology.

$$M^2_{ve}(Y^2_m(n, n)) = \sum_{x_1, x_2 \in E} (\xi_{ve}(x_1) \times \xi_{ve}(x_2))$$

$$= (25)(n) + (40)(2n) + (63)(4n) + (21)(4n) + (72)(2n) + (49)(2n) + (81)\left(\frac{9n^2}{4} - \frac{n}{2} + 18mn + 9\right)$$

$$= 729 + \frac{729n^2}{4} + (1285\frac{2}{2} + 1458m)n.$$  (16)

5.3. The Randić Index Developed by ve-Degree Methodology.

Using the edge-partition details described in the Table 3, we measured the Randić index developed by ve-degree methodology:

$$R_{ve}(Y^2_m(n, n)) = \sum_{x_1, x_2 \in E} (\xi_{ve}(x_1) \times \xi_{ve}(x_2))^{(-1/2)}$$

$$= (35)(^{-1/2})(n) + (40)(^{-1/2})(2n) + (63)(^{-1/2})(4n) + (21)(^{-1/2})(4n)$$

$$+ (72)(^{-1/2})(2n) + (49)(^{-1/2})(2n) + (81)(^{-1/2})\left(\frac{9n^2}{4} - \frac{n}{2} + 18mn + 9\right)$$

$$= 1 + \frac{n^2}{4} + \left(\frac{271\sqrt{10}}{630} + \frac{4\sqrt{7}}{21} + \frac{4\sqrt{21}}{21} + \frac{\sqrt{2}}{6} + 2m\right)n.$$  (17)

5.4. The Atom-Bond Connectivity Index Developed by ve-Degree Methodology. Utilizing the edge-partition details described in the Table 3, we measured the atom-bond connectivity index developed by ve-degree methodology:
\[
\begin{align*}
\text{Table 3: The ve-degrees of each edge of } Y^2_m(n, n). \\
(\xi(x_1), \xi(x_2)) & & (\xi_{ve}(x_1), \xi_{ve}(x_2)) & & \text{Count} \\
(2, 2) & & (5, 5) & & n \\
(2, 3) & & (5, 8) & & 2n \\
(3, 3) & & (7, 9) & & 4n \\
(1, 3) & & (3, 7) & & 4n \\
(2, 3) & & (8, 9) & & 2n \\
(3, 3) & & (7, 7) & & 2n \\
(3, 3) & & (9, 9) & & (9n^2/4) - (n/2) + 18mn + 9
\end{align*}
\]

5.5. The Geometric-Arithmetic Index Developed by ve-Degree Methodology. Utilizing the edge-partition details described in the Table 3, we measured the geometric-arithmetic index developed by ve-degree methodology:

\[
\begin{align*}
\text{GA}_{ve}(Y^2_m(n, n)) & = \sum_{x_1, x_2 \in E} \left( \frac{\xi_{ve}(x_1) \times \xi_{ve}(x_2)}{\xi_{ve}(x_1) + \xi_{ve}(x_2)} \right)^{1/2} \\
& = (n) \left( \frac{8}{25} + (2n) \frac{11}{40} + (2n) \frac{14}{63} \right) \left( \frac{8}{21} + (2n) \frac{15}{72} + (2n) \frac{12}{49} \right) + \sqrt{\frac{16}{81} \left( \frac{9n^2}{4} - \frac{n}{2} + 18mn + 9 \right)} \\
& = 4 + n^2 + \left( \frac{26\sqrt{2}}{15} + \frac{\sqrt{110}}{10} + \frac{8\sqrt{42}}{21} + \frac{\sqrt{30}}{6} + \frac{4\sqrt{3}}{7} + \frac{2}{5} + 8m \right)n \\
\end{align*}
\]  

\[
\begin{align*}
\text{ABC}_{ve}(Y^2_m(n, n)) & = \sum_{x_1, x_2 \in E} \left( \frac{\xi_{ve}(x_1) + \xi_{ve}(x_2)}{\xi_{ve}(x_1) \times \xi_{ve}(x_2)} - 2 \right)^{1/2} \\
& = (n) \left( \frac{8}{25} + (2n) \frac{11}{40} + (2n) \frac{14}{63} \right) \left( \frac{8}{21} + (2n) \frac{15}{72} + (2n) \frac{12}{49} \right) + \sqrt{\frac{16}{81} \left( \frac{9n^2}{4} - \frac{n}{2} + 18mn + 9 \right)} \\
& = 4 + n^2 + \left( \frac{26\sqrt{2}}{15} + \frac{\sqrt{110}}{10} + \frac{8\sqrt{42}}{21} + \frac{\sqrt{30}}{6} + \frac{4\sqrt{3}}{7} + \frac{2}{5} + 8m \right)n.
\end{align*}
\]
5.6. The Harmonic Index Developed by ve-Degree Methodology. Utilizing the edge-partition details described in the Table 3, we measured the harmonic index developed by ve-degree methodology:

\[ H_{ve}(Y^2_m(n,n)) = \sum_{x_i,x_j \in E} \xi_{ve}(x_1) + \xi_{ve}(x_2) \]
\[ = (n) \frac{2}{10} + (2n) \frac{2}{13} + (4n) \frac{2}{16} + (4n) \frac{2}{10} + (2n) \frac{2}{17} + (2n) \frac{2}{14} + \frac{2}{18} \left( \frac{9n^2}{4} - n + 18mn + 9 \right) \] (20)

\[ = 1 + \frac{n^2}{4} + \left( \frac{31649}{13923} + 2m \right)n. \]

5.7. The Sum-Connectivity Index Developed by ve-Degree Methodology. Utilizing the edge-partition details described in the Table 3, we measured the sum-connectivity index developed by ve-degree methodology:

\[ \chi_{ve}(Y^2_m(n,n)) = \sum_{x_i,x_j \in E} (\xi_{ve}(x_1) + \xi_{ve}(x_2))^{(-1/2)} \]
\[ = (n) \frac{1}{\sqrt{10}} + (2n) \frac{1}{\sqrt{13}} + (4n) \frac{1}{\sqrt{16}} + (4n) \frac{1}{\sqrt{10}} + (2n) \frac{1}{\sqrt{17}} + (2n) \frac{1}{\sqrt{14}} + \frac{1}{\sqrt{18}} \left( \frac{9n^2}{4} - n + 18mn + 9 \right) \] (21)
\[ = \left( \frac{\sqrt{10}}{2} + \frac{2\sqrt{13}}{13} + 1 + \frac{2\sqrt{17}}{17} + \frac{\sqrt{14}}{7} + \frac{\sqrt{2}}{6} \left( -\frac{1}{2} + 18m \right) \right)n + \frac{3\sqrt{2}n^2}{8} + \frac{\sqrt{2}}{2}. \]

6. The ve-Degree Results of Y-Junction Graph Y^3_m(n,n)

In Y^3_m(n,n) when one tube appears with exactly 2n pendants, we denote it by Y^4_m(n,n), see Figure 2. The order and size of this new graph is \((3n^2/2) + 11n + 12mn + 6\) and \((9n^2/4) + (25n/2) + 18mn + 9\), respectively. The Y-junction graph Y^3_m(n,n) is obtained by attaching 4n pendants to any two tubes of Y^2_m(n,n), see Figure 3. The cardinality of Y^2_m(n,n) is \((3n^2/2) + 13n + 12mn + 6\) and size is \((9n^2/4) + (29n/2) + 18mn + 9\). The graph Y^3_m(n,n) with maximum possible pendants denoted by Y^3_m(n,n), see Figure 4. It has order \((3n^2/2) + 15n + 12mn + 6\) and size \((9n^2/4) + (33n/2) + 18mn + 9\).

6.1. The First ve-Degree Zagreb β Index.

\[ M_{ve}^1(Y^3_m(n,n)) = \sum_{x_i,x_j \in E} (\xi_{ve}(x_1) + \xi_{ve}(x_2)) \]
\[ = (16)(6n) + (10)(6n) + (14)(3n) + (18) \left( \frac{9n^2}{4} + \frac{3n}{2} + 18mn + 9 \right) \] (22)
\[ = 162 + \frac{81n^2}{2} + (225 + 324m)n. \]
6.2. The Second Zagreb Index Developed by \(ve\)-Degree Methodology.

\[
M_{ve}^{2}(Y_{m}^{3}(n,n)) = \sum_{x_{1},x_{2} \in E} (\xi_{ve}(x_{1}) \times \xi_{ve}(x_{2}))
\]

\[
= (63)(6n) + (21)(6n) + (49)(3n) \\
+ (81)\left(\frac{9n^{2}}{4} + \frac{3n}{2} + 18mn + 9\right)
\]  

\[
= 729 + \frac{729n^{2}}{4} + \left(\frac{1545}{2} + 1458n\right)n. \tag{23}
\]

6.3. The Randić Index Developed by \(ve\)-Degree Methodology.

\[
R_{ve}(Y_{m}^{3}(n,n)) = \sum_{x_{1},x_{2} \in E} (\xi_{ve}(x_{1}) \times \xi_{ve}(x_{2}))^{-1/2}
\]

\[
= (63)^{-1/2}(6n) + (21)^{-1/2}(6n) + (49)^{-1/2}(3n) \\
+ (81)^{-1/2}\left(\frac{9n^{2}}{4} + \frac{3n}{2} + 18mn + 9\right)
\]

\[
= 1 + n^{2} + \left(\frac{2\sqrt{7}}{7} + \frac{2\sqrt{21}}{7} + \frac{25}{42} + 2m\right)n. \tag{24}
\]

6.4. The Atom-Bond Connectivity Index Developed by \(ve\)-Degree Methodology.

\[
ABC_{ve}(Y_{m}^{3}(n,n)) = \sum_{x_{1},x_{2} \in E} \left(\frac{\xi_{ve}(x_{1}) + \xi_{ve}(x_{2}) - 2}{\xi_{ve}(x_{1}) \times \xi_{ve}(x_{2})}\right)^{1/2}
\]

\[
= (6n)\sqrt{\frac{14}{63}} + (6n)\sqrt{\frac{8}{21}} + (3n)\sqrt{\frac{12}{49}} + (81)\left(\frac{9n^{2}}{4} + \frac{3n}{2} + 18mn + 9\right)
\]

\[
= 4 + n^{2} + \left(\frac{2\sqrt{2}}{7} + \frac{4\sqrt{42}}{7} + \frac{6\sqrt{3}}{7} + \frac{2}{3} + 8m\right)n. \tag{25}
\]

6.5. The Geometric-Arithmetic Index Developed by \(ve\)-Degree Methodology.

\[
ABC_{ve}(Y_{m}^{3}(n,n)) = \sum_{x_{1},x_{2} \in E} \left(\frac{\xi_{ve}(x_{1}) + \xi_{ve}(x_{2}) - 2}{\xi_{ve}(x_{1}) \times \xi_{ve}(x_{2})}\right)^{1/2}
\]

\[
= (6n)\sqrt{\frac{14}{63}} + (6n)\sqrt{\frac{8}{21}} + (3n)\sqrt{\frac{12}{49}} + (81)\left(\frac{9n^{2}}{4} + \frac{3n}{2} + 18mn + 9\right)
\]

\[
= 4 + n^{2} + \left(\frac{2\sqrt{2}}{7} + \frac{4\sqrt{42}}{7} + \frac{6\sqrt{3}}{7} + \frac{2}{3} + 8m\right)n. \tag{25}
\]
Table 4: The ve-degrees of each edge of $Y_m^3(n, n)$.

| $(\xi(x_1), \xi(x_2))$ | $(\xi_{ve}(x_1), \xi_{ve}(x_2))$ | Count |
|------------------------|---------------------------------|-------|
| (3, 3)                 | (7, 9)                          | 6n    |
| (1, 3)                 | (3, 7)                          | 6n    |
| (3, 3)                 | (7, 7)                          | 3n    |
| (3, 3)                 | (9, 9)                          | $(9n^2/4) - (3n/2) + 18n + 9$ |

Table 5: Numerical comparison of $M_{ve}^1$, $M_{ve}^2$, $H_{ve}$, $R_{ve}$, $\chi_{ve}$, $ABC_{ve}$, $GA_{ve}$ for Y-joincture graph $Y_m(n, n)$.

| (m, n) | $M_{ve}^1$ | $M_{ve}^2$ | $R_{ve}$ | $ABC_{ve}$ | $GA_{ve}$ | $H_{ve}$ | $\chi_{ve}$ |
|--------|------------|------------|----------|------------|-----------|---------|-------------|
| (5, 5) | 9919.50    | 43647.8    | 66.0289  | 256.910    | 566.888   | 65.8948 | 136.481     |
| (6, 6) | 14058.0    | 62073.0    | 92.5347  | 361.493    | 799.966   | 92.3738 | 191.992     |
| (7, 7) | 18925.5    | 83778.8    | 123.541  | 484.074    | 1073.57   | 123.353 | 257.048     |
| (8, 8) | 24522.0    | 108765.0   | 159.045  | 624.656    | 1387.62   | 158.832 | 331.649     |
| (9, 9) | 30847.5    | 137032.0   | 199.055  | 783.240    | 1742.20   | 198.811 | 415.797     |
| (10, 10)| 37902.0   | 168579.0   | 243.558  | 959.820    | 2137.28   | 243.290 | 509.491     |
| (11, 11)| 45685.5   | 203407.0   | 292.564  | 1154.40    | 2572.86   | 292.269 | 612.730     |
| (12, 12)| 54198.0   | 241515.0   | 346.069  | 1366.98    | 3048.94   | 345.748 | 725.515     |
| (13, 13)| 63439.5   | 282904.0   | 404.075  | 1597.56    | 3565.50   | 403.726 | 847.847     |
| (14, 14)| 73410.0   | 327573.0   | 466.581  | 1846.15    | 4122.58   | 466.205 | 979.737     |

Table 6: Numerical comparison of $M_{ve}^1$, $M_{ve}^2$, $H_{ve}$, $R_{ve}$, $\chi_{ve}$, $ABC_{ve}$, $GA_{ve}$ for Y-joincture graph $Y_m^3(n, n)$.

| (m, n) | $M_{ve}^1$ | $M_{ve}^2$ | $R_{ve}$ | $ABC_{ve}$ | $GA_{ve}$ | $H_{ve}$ | $\chi_{ve}$ |
|--------|------------|------------|----------|------------|-----------|---------|-------------|
| (5, 5) | 10079.5    | 44297.8    | 67.5368  | 262.078    | 576.262   | 67.2553 | 139.058     |
| (6, 6) | 14250.0    | 62853.0    | 94.3441  | 367.695    | 811.214   | 94.0065 | 195.082     |
| (7, 7) | 19149.5    | 84688.8    | 125.652  | 491.309    | 1086.66   | 125.257 | 260.653     |
| (8, 8) | 24778.0    | 109805.0   | 161.459  | 632.925    | 1402.61   | 161.008 | 335.770     |
| (9, 9) | 31135.5    | 138202.0   | 201.767  | 792.543    | 1759.08   | 201.259 | 420.433     |
| (10, 10)| 38222.0   | 169879.0   | 246.574  | 970.157    | 2156.02   | 246.011 | 514.641     |
| (11, 11)| 46037.5   | 204837.0   | 295.881  | 1165.77    | 2593.47   | 295.262 | 618.397     |
| (12, 12)| 54582.0   | 243075.0   | 349.688  | 1379.39    | 3071.43   | 349.013 | 731.697     |
| (13, 13)| 63855.5   | 284594.0   | 407.996  | 1611.00    | 3589.89   | 407.264 | 854.543     |
| (14, 14)| 73858.0   | 329393.0   | 470.803  | 1860.62    | 4148.83   | 470.015 | 986.937     |

\[
GA_{ve}(Y_m^3(n, n)) = \sum_{x_1, x_2 \in E} \frac{2(\xi_{ve}(x_1) \times \xi_{ve}(x_2))^{1/2}}{\xi_{ve}(x_1) + \xi_{ve}(x_2)}
\]

(26)

\[
= (6n) \frac{(2)\sqrt{63}}{16} + (6n) \frac{(2)\sqrt{21}}{10} + (3n) \frac{(2)\sqrt{49}}{14} + (2)\sqrt{81} \frac{9n^2}{4} + \frac{3n}{2} + 18mn + 9
\]

\[
= 9 + \frac{9n^2}{4} + \left(\frac{9\sqrt{7}}{4} + \frac{6\sqrt{21}}{5} + \frac{9}{2} + 18m\right)n.
\]

6.6. The Harmonic Index Developed by ve-Degree Methodology. Utilizing the edge-partition details described in the Table 4, we measured the harmonic index developed by ve-degree methodology:
\[ H_{ve}(Y^m_n(n,n)) = \sum_{x_1, x_2 \in E} \left( \xi_{ve}(x_1) + \xi_{ve}(x_2) \right) \]

\[ = (6n)^2 \frac{2}{16} + (6n)^2 \frac{2}{10} + (3n)^2 \frac{2}{14} \left( \frac{9n^2}{4} + \frac{3n}{2} + 18mn + 9 \right) \]

\[ = 1 + \frac{n^2}{4} + \left( \frac{1069}{420} + 2m \right)n. \]  

(27)

\[ \chi_{ve}(Y^m_n(n,n)) = \sum_{x_1, x_2 \in E} \left( \xi_{ve}(x_1) + \xi_{ve}(x_2) \right)^{-1/2} \]

\[ = (6n)^2 \frac{1}{\sqrt{16}} + (6n)^2 \frac{1}{\sqrt{10}} + (3n)^2 \frac{1}{\sqrt{14}} \left( \frac{9n^2}{4} + \frac{3n}{2} + 18mn + 9 \right) \]

\[ = 3 \sqrt{2}n^2 \frac{3}{8} + \left( \frac{3}{2} + \frac{3 \sqrt{10}}{5} + \frac{3 \sqrt{14}}{14} + \frac{\sqrt{2}}{6} \frac{3}{2} + 18m \right)n + 3 \sqrt{2} \div 2. \quad \]  

(28)

7. Conclusion

In this research work, ve-degree topological indices are measured of Y-junctions and their three different variants. We determined the first ve-degree Zagreb \( \beta \)-index, second Zagreb index, Randić, atom-bond-connectivity index, general sum-connectivity and geometric-arithmetic, and harmonic index developed by ve-degree methodology, for four types of Y-shaped carbon nanotube junctions \( Y^m_n(n,n) \). The results of Y-junctions and their structures are also elaborated

6.7. The Sum-Connectivity Index Developed by ve-Degree Methodology. Utilizing the edge-partition details described in the Table 4, we measured the sum-connectivity index developed by ve-degree methodology:

\[ H_{ve}(Y^3_n(n,n)) = \sum_{x_1, x_2 \in E} \left( \xi_{ve}(x_1) + \xi_{ve}(x_2) \right) \]

\[ = (6n)^2 \frac{2}{16} + (6n)^2 \frac{2}{10} + (3n)^2 \frac{2}{14} \left( \frac{9n^2}{4} + \frac{3n}{2} + 18mn + 9 \right) \]

\[ = 1 + \frac{n^2}{4} + \left( \frac{1069}{420} + 2m \right)n. \]  

(27)
in numerical Tables 5–8. Instead of a whole complex structure, it will be easy to see as a numeric quantity.

**Data Availability**

There is not data associative with this manuscript.

**Conflicts of Interest**

The author declares that he has no conflicts of interest.

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