COMPUTATION AND ANALYSIS OF VICINAL DEGREE-BASED TOPOLOGICAL INDICES OF CARBON NANOTUBES

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Abstract: In computational chemistry, the characteristics of a molecular compound can be evaluated with the help of a numerical value, known as a topological index. Topological indices are extensively used to study the molecular mechanics in QSAR and QSPR analysis. In this study, we introduced the vicinal degree and vicinal degree-based topological indices such as geometric-arithmetic vicinal index, atom bond connectivity vicinal index, harmonic vicinal index, inverse sum indeg vicinal index, Randić vicinal index, and sum-connectivity vicinal index for planar polyhex zigzag carbon nanotubes, where these carbon nanotubes (CNTs) are nanomaterials with broad applications that are produced on a large scale. Furthermore, we verify the correlation between the general degree-based topological indices and the vicinal degree-based topological indices, and the R code for finding these vicinal topological indices.

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1. Introduction:

The structural or physicochemical property of a molecule plays a significant role in chemistry, pharmacology, etc. The study of these molecular compounds in terms of a simple connected planar graph is a branch of graph theory known as chemical graph theory. The vertices of a chemical graph are the atoms of the compounds, and the edges represent the bonds between the atoms, and the hydrogen atoms are often omitted, referred from book by D Bonchev [1]. The degree of the vertex is the number of edges incident with that vertex; on the other hand, the degree of a vertex is the valency of the atom in chemical graph theory.

To study the properties of a chemical compound and predict certain physicochemical properties like boiling point, molecular weight, density, entropy, refractive index, and so forth, a numerical quantity called the topological index can be used. The chemist Harold Wiener created the Wiener index, the most well-known topological descriptor, in 1947 and utilized it to ascertain the physical characteristics of several alkane kinds known as paraffin [2]. This marked the beginning of the study of topological indices in chemistry. Additionally, the mathematical models that can be used to predict the chemical, physical, or biological aspects of chemical compounds are the quantitative structure-activity relationship (QSAR) and the quantitative structure-property relationship (QSPR) [3].

Researchers have demonstrated that carbon nanotubes (CNTs) can be used for drug and biomolecule transport, tumor imaging, and photothermal therapy. Iijima made the first observation of carbon nanotubes (CNTs) in 1991. CNTs are distinguished by their hollow, nanoscale tubes [4]. CNTs fall into the realm of inorganic chemistry. Based on the number of layers, CNTs can be classified as either single-walled carbon nanotubes (SWCNTs) or multiple-walled carbon nanotubes (MWCNTs). For different topological indices of different structures of nanotubes, we recommend the following articles [5-19]. Both SWCNTs and MWCNTs are popular nanomaterials for commercial applications and widely used in fuel cell designs, photovoltaics, and biomedicine. Depending on how the graphite is rolled up, for these two different basic structures, there are three different possible types of CNTs. Armchair carbon nanotubes, zigzag carbon nanotubes, and chiral carbon nanotubes are these three varieties of CNTs. For more applications on CNTs, we recommend the following articles [20-24].

2. Preliminaries:

In this paper, we consider only finite, simple, connected graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of edges incident with v.

2.1 Vicinal degree of a vertex:

The vicinal degree of a vertex $u \in V(G)$ denoted by $\nu\iota(u)$ is defined as,

$$\nu\iota(u) = \left(\sum_{u_i \in N(u)} \mathrm{d}_G(u_i) \right) - d_G(u) \qquad (1)$$

Where $N(u)$ is the open neighbourhood set of vertex u.

2.2 Vicinal topological indices:

We introduced some vicinal degree based topological indices as follows:

Furtula & Vukicevic [25] introduced the geometric-arithmetic index (GA), In this study we have defined its new version called geometric-arithmetic vicinal index as follows:

$$GA_{\nu\iota}(G) = \sum_{u_1u_2 \in E(G)} \frac{2\sqrt{\nu\iota(u_1)\nu\iota(u_2)}}{\nu\iota(u_1)+\nu\iota(u_2)} \qquad (2)$$

Das, Gutman, & Furtula [26] introduced the atom bond connectivity index (ABC), in this study we have defined its new version called atom bond connectivity vicinal index as follows:

$$ABC_{\nu\iota}(G) = \sum_{u_1u_2 \in E(G)} \sqrt{\frac{\nu\iota(u_1)+\nu\iota(u_2)-2}{\nu\iota(u_1)\nu\iota(u_2)}} \qquad (3)$$

Zhong [27] introduced the harmonic index (H), in this study we have defined its new version called harmonic vicinal index as follows:

$$H_{\nu\iota}(G) = \sum_{u_1u_2 \in E(G)} \frac{2}{\nu\iota(u_1)+\nu\iota(u_2)} \qquad (4)$$

Pattabiraman [28] introduced the inverse sum indeg index (ISI), in this study we have defined its new version called inverse sum indeg vicinal index as follows:

$$ISI_{\nu\iota}(G) = \sum_{u_1u_2 \in E(G)} \frac{\nu\iota(u_1)\nu\iota(u_2)}{\nu\iota(u_1)+\nu\iota(u_2)} \qquad (5)$$

Randić [29] introduced the Randić index (R) in 1975, in this study we have defined its new version called Randić vicinal index as follows:

$$R_{\nu\iota}(G) = \sum_{u_1u_2 \in E(G)} \frac{1}{\sqrt{\nu\iota(u_1)\nu\iota(u_2)}} \qquad (6)$$

Zhou & Trinajstić [30] introduced the sum-connectivity index (SCI) in 2009, in this study we have defined its new version called sum-connectivity vicinal index as follows:

$$SCI_{\nu\iota}(G) = \sum_{u_1u_2 \in E(G)} \frac{1}{\sqrt{\nu\iota(u_1)+\nu\iota(u_2)}} \qquad (7)$$

2.3 Structure of planar polyhex zigzag nanotubes $PTUZC_6[m,n]$:

The planar polyhex zigzag nanotubes $PTUZC_6[m,n]$, where m and n are the number of hexagons in the first row/column of the 2-dimensional lattice as shown in fig.1, where $m,n > 1$.

The total number of vertices and total number of edges of $PTUZC_6[m,n]$ are $2n(2m+1)$ and $6nm+n-m$, respectively. [31]

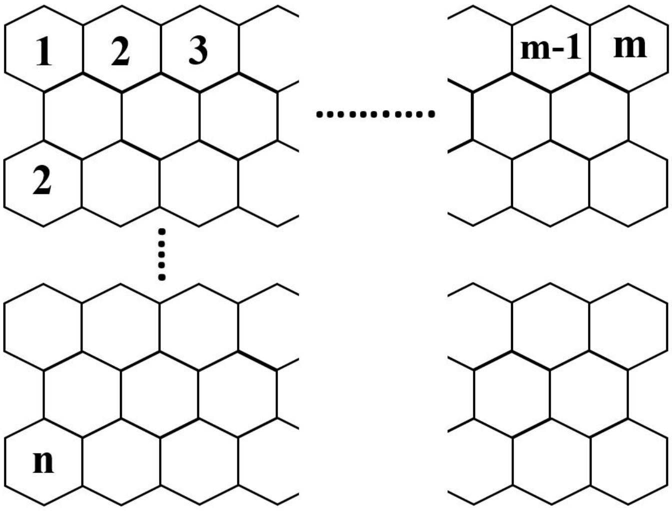


Figure 1. 2-Dimensional lattice of planar polyhex zigzag nanotube $PTUZC_6[m,n]$.

Let G be a graph of planar polyhex zigzag nanotube $PTUZC_6[m,n]$.

Using equation (1), in *G* there are five types of vertices and nine types of edges based on the vicinal degree as shown in Table 1 and Table 2, respectively. Where,

$$IE_{(i,j)} = \{uv \in E(G) \mid v\iota(u) = i \,\&\, v\iota(v) = j\}$$
$$IV_i = \{v \in V(G) \mid v\iota(v) = i\}$$

$\lvert IV_2\rvert$	$\lvert IV_3\rvert$	$\lvert IV_4\rvert$	$\lvert IV_5\rvert$	$\lvert IV_6\rvert$
4	$4n$	$4m-6$	$4(n-1)$	$2(n-1)(2m-3)$

Table 1. Vertex partition based on vicinal degree.

$\lvert IE_{(2,3)}\rvert$	$\lvert IE_{(3,4)}\rvert$	$\lvert IE_{(3,5)}\rvert$	$\lvert IE_{(3,3)}\rvert$	$\lvert IE_{(4,6)}\rvert$	$\lvert IE_{(4,4)}\rvert$	$\lvert IE_{(5,6)}\rvert$	$\lvert IE_{(5,5)}\rvert$	$\lvert IE_{(6,6)}\rvert$
8	4	$4(n-1)$	$2(n-2)$	$2(m-1)$	$4(m-2)$	$4(n-1)$	$2(n-1)$	$6mn-7m-11n+1$

Table 2. Edge partition based on vicinal degree.

3. Theorem: Let G be Planar Polyhex zigzag nanotube $PTUZC_6[m,n]$ where $m,n>1$ then,

1. $GA_{v\iota}(G) = 6mn - 3m + 0.86n + 3.90$
2. $ABC_{v\iota}(G) = 3.16mn - 0.09m + 1.39n + 0.56$
3. $H_{v\iota}(G) = mn + 0.23m + 0.96n + 0.48$
4. $ISI_{v\iota}(G) = 18nm - 8.20m - 6.59n + 2.25$
5. $R_{v\iota}(G) = mn + 0.24m + n + 0.52$
6. $SCI_{v\iota}(G) = 1.73mn + 0.02m + 0.89n + 0.21$

Proof. Let G be the graph $PTUZC_6[m,n]$. Then using Table 1. We deduce,

1. To compute geometric-arithmetic vicinal index of G i.e. $GA_{vi}(G)$ using equation (2) is,

$$GA_{vi}(G)=\sum_{u_1u_2\in E(G)}\frac{2\sqrt{vi(u_1)vi(u_2)}}{vi(u_1)+vi(u_2)}$$
$$=\sum_{IE_{(2,3)}}\frac{2\sqrt{vi(u_1)vi(u_2)}}{vi(u_1)+vi(u_2)}+\sum_{IE_{(3,4)}}\frac{2\sqrt{vi(u_1)vi(u_2)}}{vi(u_1)+vi(u_2)}+\sum_{IE_{(3,5)}}\frac{2\sqrt{vi(u_1)vi(u_2)}}{vi(u_1)+vi(u_2)}+\sum_{IE_{(3,3)}}\frac{2\sqrt{vi(u_1)vi(u_2)}}{vi(u_1)+vi(u_2)}+\sum_{IE_{(4,6)}}\frac{2\sqrt{vi(u_1)vi(u_2)}}{vi(u_1)+vi(u_2)}$$
$$+\sum_{IE_{(4,4)}}\frac{2\sqrt{vi(u_1)vi(u_2)}}{vi(u_1)+vi(u_2)}+\sum_{IE_{(5,6)}}\frac{2\sqrt{vi(u_1)vi(u_2)}}{vi(u_1)+vi(u_2)}+\sum_{IE_{(5,5)}}\frac{2\sqrt{vi(u_1)vi(u_2)}}{vi(u_1)+vi(u_2)}+\sum_{IE_{(6,6)}}\frac{2\sqrt{vi(u_1)vi(u_2)}}{vi(u_1)+vi(u_2)}$$
$$=8\left(\frac{2\sqrt{2\times3}}{2+3}\right)+4\left(\frac{2\sqrt{3\times4}}{3+4}\right)+4(n-1)\left(\frac{2\sqrt{3\times5}}{3+5}\right)+2(n-2)\left(\frac{2\sqrt{3\times3}}{3+3}\right)+2(m-1)\left(\frac{2\sqrt{4\times6}}{4+6}\right)$$
$$+4(m-2)\left(\frac{2\sqrt{4\times4}}{4+4}\right)+4(n-1)\left(\frac{2\sqrt{5\times6}}{5+6}\right)+2(n-1)\left(\frac{2\sqrt{5\times5}}{5+5}\right)+(6mn-7m-11n+12)\left(\frac{2\sqrt{6\times6}}{6+6}\right)$$

$$=13.76+9.86(n-1)+2(n-2)+4(m-2)+5(m-2)(n-1)+(m-1)(n-2)$$
$$GA_{vi}(G)=6mn-3m+0.86n+3.90$$

2. To compute atom bond connectivity vicinal index of a graph G i.e. $ABC_{vi}(G)$ using equation (3) is,

$$ABC_{vi}(G)=\sum_{u_1u_2\in E(G)}\sqrt{\frac{vi(u_1)+vi(u_2)-2}{vi(u_1)vi(u_2)}}$$
$$=\sum_{IE_{(2,3)}}\sqrt{\frac{vi(u_1)+vi(u_2)-2}{vi(u_1)vi(u_2)}}+\sum_{IE_{(3,4)}}\sqrt{\frac{vi(u_1)+vi(u_2)-2}{vi(u_1)vi(u_2)}}+\sum_{IE_{(3,5)}}\sqrt{\frac{vi(u_1)+vi(u_2)-2}{vi(u_1)vi(u_2)}}+\sum_{IE_{(3,3)}}\sqrt{\frac{vi(u_1)+vi(u_2)-2}{vi(u_1)vi(u_2)}}+\sum_{IE_{(4,6)}}\sqrt{\frac{vi(u_1)+vi(u_2)-2}{vi(u_1)vi(u_2)}}$$
$$+\sum_{IE_{(4,4)}}\sqrt{\frac{vi(u_1)+vi(u_2)-2}{vi(u_1)vi(u_2)}}+\sum_{IE_{(5,6)}}\sqrt{\frac{vi(u_1)+vi(u_2)-2}{vi(u_1)vi(u_2)}}+\sum_{IE_{(5,5)}}\sqrt{\frac{vi(u_1)+vi(u_2)-2}{vi(u_1)vi(u_2)}}+\sum_{IE_{(6,6)}}\sqrt{\frac{vi(u_1)+vi(u_2)-2}{vi(u_1)vi(u_2)}}$$
$$=8\left(\sqrt{\frac{2+3-2}{2\times3}}\right)+4\left(\sqrt{\frac{3+4-2}{3\times4}}\right)+4(n-1)\left(\sqrt{\frac{3+5-2}{3\times5}}\right)+2(n-2)\left(\sqrt{\frac{3+3-2}{3\times3}}\right)+2(m-1)\left(\sqrt{\frac{4+6-2}{4\times6}}\right)$$
$$+4(m-2)\left(\sqrt{\frac{4+4-2}{4\times4}}\right)+4(n-1)\left(\sqrt{\frac{5+6-2}{5\times6}}\right)+2(n-1)\left(\sqrt{\frac{5+5-2}{5\times5}}\right)+(6mn-7m-11n+12)\left(\sqrt{\frac{6+6-2}{6\times6}}\right)$$
$$=5.85n-5.85+1.33n-2.67+1.15m-1.15+2.45m-4.90+3.16nm-3.69m-5.80n+6.32$$
$$ABC_{vi}(G)=3.16mn-0.09m+1.39n+0.56$$

3. To compute Harmonic vicinal index of a graph G i.e. $H_{\nu\iota}(G)$ using equation (4) is,

$$H_{\nu\iota}(G)=\sum_{u_1u_2\in E(G)}\frac{2}{\nu\iota(u_1)+\nu\iota(u_2)}$$

$$=\sum_{IE_{(2,3)}}\frac{2}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(3,4)}}\frac{2}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(3,5)}}\frac{2}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(3,3)}}\frac{2}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(4,6)}}\frac{2}{\nu\iota(u_1)+\nu\iota(u_2)}$$

$$+\sum_{IE_{(4,4)}}\frac{2}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(5,6)}}\frac{2}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(5,5)}}\frac{2}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(6,6)}}\frac{2}{\nu\iota(u_1)+\nu\iota(u_2)}$$

$$=8\left(\frac{2}{2+3}\right)+4\left(\frac{2}{3+4}\right)+4(n-1)\left(\frac{2}{3+5}\right)+2(n-2)\left(\frac{2}{3+3}\right)+2(m-1)\left(\frac{2}{4+6}\right)$$

$$+4(m-2)\left(\frac{2}{4+4}\right)+4(n-1)\left(\frac{2}{5+6}\right)+2(n-1)\left(\frac{2}{5+5}\right)+(6mn-7m-11n+12)\left(\frac{2}{6+6}\right)$$

$$=\left(\frac{117}{55}+\frac{2}{3}-\frac{11}{6}\right)n+\left(\frac{2}{5}+1-\frac{7}{6}\right)m+nm+\left(\frac{16}{5}+\frac{8}{7}+2-\frac{117}{55}-\frac{4}{3}-\frac{2}{5}-2\right)n$$

$$H_{\nu\iota}(G)=mn+0.23m+0.96n+0.48$$

4. To compute inverse sum indeg vicinal index of a graph G i.e. $ISI_{\nu\iota}(G)$ using equation (5) is,

$$ISI_{\nu\iota}(G)=\sum_{u_1u_2\in E(G)}\frac{\nu\iota(u_1)\nu\iota(u_2)}{\nu\iota(u_1)+\nu\iota(u_2)}$$

$$=\sum_{IE_{(2,3)}}\frac{\nu\iota(u_1)\nu\iota(u_2)}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(3,4)}}\frac{\nu\iota(u_1)\nu\iota(u_2)}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(3,5)}}\frac{\nu\iota(u_1)\nu\iota(u_2)}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(3,3)}}\frac{\nu\iota(u_1)\nu\iota(u_2)}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(4,6)}}\frac{\nu\iota(u_1)\nu\iota(u_2)}{\nu\iota(u_1)+\nu\iota(u_2)}$$

$$+\sum_{IE_{(4,4)}}\frac{\nu\iota(u_1)\nu\iota(u_2)}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(5,6)}}\frac{\nu\iota(u_1)\nu\iota(u_2)}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(5,5)}}\frac{\nu\iota(u_1)\nu\iota(u_2)}{\nu\iota(u_1)+\nu\iota(u_2)}+\sum_{IE_{(6,6)}}\frac{\nu\iota(u_1)\nu\iota(u_2)}{\nu\iota(u_1)+\nu\iota(u_2)}$$

$$=8\left(\frac{2\times 3}{2+3}\right)+4\left(\frac{3\times 4}{3+4}\right)+4(n-1)\left(\frac{3\times 5}{3+5}\right)+2(n-2)\left(\frac{3\times 3}{3+3}\right)+2(m-1)\left(\frac{4\times 6}{4+6}\right)$$

$$+4(m-2)\left(\frac{4\times 4}{4+4}\right)+4(n-1)\left(\frac{5\times 6}{5+6}\right)+2(n-1)\left(\frac{5\times 5}{5+5}\right)+(6mn-7m-11n+12)\left(\frac{6\times 6}{6+6}\right)$$

$$=16.46+23.41n-23.41+3n-6+4.80m-4.80+8m-16+8nm-21m-33n+36$$

$$ISI_{\nu\iota}(G)=18nm-8.20m-6.59n+2.25$$

5. To compute Randić vicinal index of a graph G i.e. $R_{\nu\iota}(G)$ using equation (6) is,

$$R_{\nu\iota}(G)=\sum_{u_1u_2\in E(G)}\frac{1}{\sqrt{\nu\iota(u_1)\nu\iota(u_2)}}$$

$$=\sum_{IE_{(2,3)}}\frac{1}{\sqrt{\nu\iota(u_1)\nu\iota(u_2)}}+\sum_{IE_{(3,4)}}\frac{1}{\sqrt{\nu\iota(u_1)\nu\iota(u_2)}}+\sum_{IE_{(3,5)}}\frac{1}{\sqrt{\nu\iota(u_1)\nu\iota(u_2)}}+\sum_{IE_{(3,3)}}\frac{1}{\sqrt{\nu\iota(u_1)\nu\iota(u_2)}}+\sum_{IE_{(4,6)}}\frac{1}{\sqrt{\nu\iota(u_1)\nu\iota(u_2)}}$$

$$+\sum_{IE_{(4,4)}}\frac{1}{\sqrt{\nu\iota(u_1)\nu\iota(u_2)}}+\sum_{IE_{(5,6)}}\frac{1}{\sqrt{\nu\iota(u_1)\nu\iota(u_2)}}+\sum_{IE_{(5,5)}}\frac{1}{\sqrt{\nu\iota(u_1)\nu\iota(u_2)}}+\sum_{IE_{(6,6)}}\frac{1}{\sqrt{\nu\iota(u_1)\nu\iota(u_2)}}$$

$$=8\left(\frac{1}{\sqrt{2\times3}}\right)+4\left(\frac{1}{\sqrt{3\times4}}\right)+4(n-1)\left(\frac{1}{\sqrt{3\times5}}\right)+2(n-2)\left(\frac{1}{\sqrt{3\times3}}\right)+2(m-1)\left(\frac{1}{\sqrt{4\times6}}\right)$$

$$+4(m-2)\left(\frac{1}{\sqrt{4\times4}}\right)+4(n-1)\left(\frac{1}{\sqrt{5\times6}}\right)+2(n-1)\left(\frac{1}{\sqrt{5\times5}}\right)+(6mn-7m-11n+12)\left(\frac{1}{\sqrt{6\times6}}\right)$$

$$=(2.16+0.67-1.83)n+(0.41+1-1.16)m+nm+(4.42-2.16-1.33-0.41-2+2)$$

$$R_{\nu\iota}(G)=mn+0.24m+n+0.52$$

6. To compute sum-Connectivity vicinal index of a graph G i.e. $SCI_{\nu\iota}(G)$ using equation (7) is,

$$SCI_{\nu\iota}(G)=\sum_{u_1u_2\in E(G)}\frac{1}{\sqrt{\nu\iota(u_1)+\nu\iota(u_2)}}$$

$$=\sum_{IE_{(2,3)}}\frac{1}{\sqrt{\nu\iota(u_1)+\nu\iota(u_2)}}+\sum_{IE_{(3,4)}}\frac{1}{\sqrt{\nu\iota(u_1)+\nu\iota(u_2)}}+\sum_{IE_{(3,5)}}\frac{1}{\sqrt{\nu\iota(u_1)+\nu\iota(u_2)}}+\sum_{IE_{(3,3)}}\frac{1}{\sqrt{\nu\iota(u_1)+\nu\iota(u_2)}}+\sum_{IE_{(4,6)}}\frac{1}{\sqrt{\nu\iota(u_1)+\nu\iota(u_2)}}$$

$$+\sum_{IE_{(4,4)}}\frac{1}{\sqrt{\nu\iota(u_1)+\nu\iota(u_2)}}+\sum_{IE_{(5,6)}}\frac{1}{\sqrt{\nu\iota(u_1)+\nu\iota(u_2)}}+\sum_{IE_{(5,5)}}\frac{1}{\sqrt{\nu\iota(u_1)+\nu\iota(u_2)}}+\sum_{IE_{(6,6)}}\frac{1}{\sqrt{\nu\iota(u_1)+\nu\iota(u_2)}}$$

$$=8\left(\frac{1}{\sqrt{2+3}}\right)+4\left(\frac{1}{\sqrt{3+4}}\right)+4(n-1)\left(\frac{1}{\sqrt{3+5}}\right)+2(n-2)\left(\frac{1}{\sqrt{3+3}}\right)+2(m-1)\left(\frac{1}{\sqrt{4+6}}\right)$$

$$+4(m-2)\left(\frac{1}{\sqrt{4+4}}\right)+4(n-1)\left(\frac{1}{\sqrt{5+6}}\right)+2(n-1)\left(\frac{1}{\sqrt{5+5}}\right)+(6mn-7m-11n+12)\left(\frac{1}{\sqrt{6+6}}\right)$$

$$=(3.25+0.82-3.18)n+(0.63+1.41-2.02)m+1.73nm+(5.09-3.25-1.64-0.63-2.82+3.46)$$

$$SCI_{\nu\iota}(G)=1.73mn+0.02m+0.89n+0.21$$

2.2 Comparison:

Here, we give a numerical and graphical representation of the vicinal topological indices,

Sr.No.	$[m,n]$	GA	$GA_{\nu\iota}$	ABC	$ABC_{\nu\iota}$	H	$H_{\nu\iota}$
1	[2,2]	23.84	23.62	16.64	6.97	9.87	6.86
3	[3,3]	53.68	51.48	37.04	24.06	20.74	13.05
3	[4,4]	95.52	91.34	65.44	47.47	35.61	21.24
4	[5,5]	149.36	143.2	101.84	77.2	54.48	31.43
5	[6,6]	215.2	207.06	146.24	113.25	77.35	43.62
6	[7,7]	293.04	282.92	198.64	155.62	104.22	57.81
7	[8,8]	382.88	370.78	259.04	204.31	135.09	74
8	[9,9]	484.72	470.64	327.44	259.32	169.96	92.19
9	[10,10]	598.56	582.5	403.84	320.65	208.83	112.38
10	[11,12]	791.32	773.22	533.14	424.44	274.63	146.53
11	[13,14]	1091	1068.94	733.94	585.02	376.37	198.91
12	[15,16]	1438.68	1412.66	966.74	770.88	494.11	259.29
13	[17,18]	1834.36	1804.38	1231.54	982.02	627.85	327.67
14	[19,20]	2278.04	2244.1	1528.34	1218.44	777.59	404.05

15	[21,22]	2769.72	2731.82	1857.14	1480.14	943.33	488.43
16	[23,24]	3309.4	3267.54	2217.94	1767.12	1125.07	580.81
17	[25,26]	3897.08	3851.26	2610.74	2079.38	1322.81	681.19
18	[27,28]	4532.76	4482.98	3035.54	2416.92	1536.55	789.57
19	[29,30]	5216.44	5162.7	3492.34	2779.74	1766.29	905.95
20	[32,31]	5946.12	5886.56	3979.74	3166.37	2011.04	1029.6
21	[34,33]	6725.8	6662.28	4500.54	3579.75	2272.78	1161.98
22	[36,35]	7553.48	7486	5053.34	4018.41	2550.52	1302.36
23	[38,37]	8429.16	8357.72	5638.14	4482.35	2844.26	1450.74
24	[40,39]	9352.84	9277.44	6254.94	4971.57	3154	1607.12
25	[42,41]	10324.52	10245.16	6903.74	5486.07	3479.74	1771.5
26	[44,43]	11344.2	11260.88	7584.54	6025.85	3821.48	1943.88
27	[46,45]	12411.88	12324.6	8297.34	6590.91	4179.22	2124.26
28	[48,47]	13527.56	13436.32	9042.14	7181.25	4552.96	2312.64
29	[50,49]	14691.24	14596.04	9818.94	7796.87	4942.7	2509.02
30	[51,53]	16211.84	16114.48	10834.04	8601.78	5452.36	2766.09
31	[54,56]	18137.36	18034.06	12119.24	9620.01	6096.97	3090.66
32	[57,59]	20170.88	20061.64	13476.44	10695.12	6777.58	3433.23
33	[60,62]	22312.4	22197.22	14905.64	11827.11	7494.19	3793.8
34	[60,60]	21590.56	21475.5	14423.84	11445.15	7252.33	3671.88
35	[63,65]	24561.92	24440.8	16406.84	13015.98	8246.8	4172.37
36	[66,68]	26919.44	26792.38	17980.04	14261.73	9035.41	4568.94
37	[69,71]	29384.96	29251.96	19625.24	15564.36	9860.02	4983.51
38	[74,72]	31954.48	31811.82	21339.64	16920.93	10718.65	5414.62
39	[77,75]	34636	34487.4	23128.84	18337.32	11615.26	5865.19
40	[80,78]	37425.52	37270.98	24990.04	19810.59	12547.87	6333.76
41	[83,81]	40323.04	40162.56	26923.24	21340.74	13516.48	6820.33
42	[81,81]	39353.2	39196.56	26276.24	20829	13192.6	6657.87
43	[86,84]	43328.56	43162.14	28928.44	22927.77	14521.09	7324.9
44	[89,87]	46442.08	46269.72	31005.64	24571.68	15561.7	7847.47
45	[90,93]	50208.52	50033.88	33518.54	26561.19	16821.22	8480.46
46	[94,97]	54695.88	54513.32	36512.14	28930.03	18320.7	9233.22
47	[98,100]	58786.32	58595.9	39240.84	31088.93	19687.25	9919.02
48	[101,104]	63010.76	62814.34	42058.94	33318.82	21098.79	10627.55
49	[105,108]	68026.12	67821.78	45404.54	35965.74	22774.27	11468.31
50	[112,109]	73227.48	73009.64	48873.94	38709.37	24510.78	12338.88
51	[116,113]	78626.84	78401.08	52475.54	41558.53	26314.26	13243.64
52	[120,117]	84218.2	83984.52	56205.14	44508.81	28181.74	14180.4
53	[115,115]	79331.76	79107.8	52945.84	41931.1	26550.18	13362.33
54	[121,126]	91461.4	91225.26	61036.74	48332.1	30602.05	15395.27
55	[127,131]	99805.52	99557.56	66602.24	52734.02	33388.34	16792.45
56	[138,132]	109268.6	108999.4	72913.64	57724.05	36546.61	18374.94
57	[145,139]	120901.4	120618.4	80672.44	63860.32	40430.7	20322.27
58	[146,156]	136642	136356.1	91171.24	72166.05	45688.45	22959.82
59	[157,167]	157298.2	156990.5	104947.6	83060.12	52584.02	26415.91
60	[178,168]	179386.5	179038.4	119678	94704.21	59953.69	30106.7

61	[180,179]	193290.4	192937.8	128950.9	102037.8	64595.8	32433.72
62	[182,182]	198715	198358.4	132568.6	104898.4	66406.47	33341.06
63	[181,195]	211754.1	211398.6	141264.8	111776.8	70760.62	35524.31
64	[200,196]	235164.5	234772.5	156876.2	124116.2	78570.41	39434.64

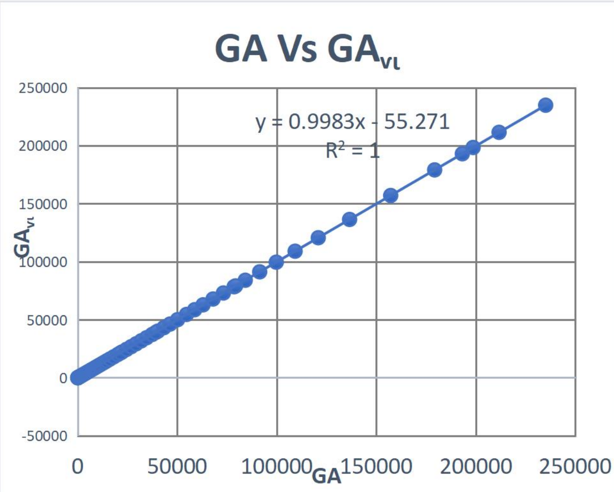
Table 3. Numerical representation of GA, $GA_{v\iota}$, ABC, $ABC_{v\iota}$, H, and $H_{v\iota}$

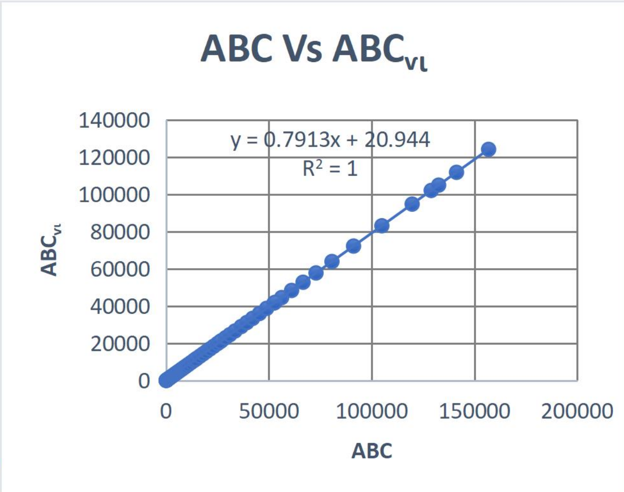
Sr.No.	$[m,n]$	ISI	$ISI_{v\iota}$	R	$R_{v\iota}$	SCI	$SCI_{v\iota}$
1	[2,2]	29.6	44.67	9.92	7	10.79	8.95
2	[3,3]	71.2	119.88	20.85	13.24	23.48	18.51
3	[4,4]	130.8	231.09	35.78	21.48	41.05	31.53
4	[5,5]	208.4	378.3	54.71	31.72	63.5	48.01
5	[6,6]	304	561.51	77.64	43.96	90.83	67.95
6	[7,7]	417.6	780.72	104.57	58.2	123.04	91.35
7	[8,8]	549.2	1035.93	135.5	74.44	160.13	118.21
8	[9,9]	698.8	1327.14	170.43	92.68	202.1	148.53
9	[10,10]	866.4	1654.35	209.36	112.92	248.95	182.31
10	[11,12]	1150.3	2208.97	275.25	147.16	328.26	239.47
11	[13,14]	1593.5	3079.39	377.11	199.64	451.24	327.79
12	[15,16]	2108.7	4093.81	494.97	260.12	593.74	429.95
13	[17,18]	2695.9	5252.23	628.83	328.6	755.76	545.95
14	[19,20]	3355.1	6554.65	778.69	405.08	937.3	675.79
15	[21,22]	4086.3	8001.07	944.55	489.56	1138.36	819.47
16	[23,24]	4889.5	9591.49	1126.41	582.04	1358.94	976.99
17	[25,26]	5764.7	11325.91	1324.27	682.52	1599.04	1148.35
18	[27,28]	6711.9	13204.33	1538.13	791	1858.66	1333.55
19	[29,30]	7731.1	15226.75	1767.99	907.48	2137.8	1532.59
20	[32,31]	8820.3	17391.56	2012.86	1031.2	2435.47	1744.6
21	[34,33]	9983.5	19701.98	2274.72	1163.68	2753.65	1971.32
22	[36,35]	11218.7	22156.4	2552.58	1304.16	3091.35	2211.88
23	[38,37]	12525.9	24754.82	2846.44	1452.64	3448.57	2466.28
24	[40,39]	13905.1	27497.24	3156.3	1609.12	3825.31	2734.52
25	[42,41]	15356.3	30383.66	3482.16	1773.6	4221.57	3016.6
26	[44,43]	16879.5	33414.08	3824.02	1946.08	4637.35	3312.52
27	[46,45]	18474.7	36588.5	4181.88	2126.56	5072.65	3622.28
28	[48,47]	20141.9	39906.92	4555.74	2315.04	5527.47	3945.88
29	[50,49]	21881.1	43369.34	4945.6	2511.52	6001.81	4283.32
30	[51,53]	24152.6	47888.78	5455.41	2768.76	6621.84	4724.59
31	[54,56]	27031.4	53622.41	6100.2	3093.48	7406.55	5282.65
32	[57,59]	30072.2	59680.04	6780.99	3436.2	8235.18	5871.85
33	[60,62]	33275	66061.67	7497.78	3796.92	9107.73	6492.19
34	[60,60]	32196.4	63914.85	7255.86	3674.92	8813.45	6282.81
35	[63,65]	36639.8	72767.3	8250.57	4175.64	10024.2	7143.67
36	[66,68]	40166.6	79796.93	9039.36	4572.36	10984.59	7826.29
37	[69,71]	43855.4	87150.56	9864.15	4987.08	11988.9	8540.05
38	[74,72]	47702.2	94824.97	10722.96	5418.28	13035.15	9283.21

39	[77,75]	51715	102826.6	11619.75	5869	14127.3	10059.25
40	[80,78]	55889.8	111152.2	12552.54	6337.72	15263.37	10866.43
41	[83,81]	60226.6	119801.9	13521.33	6824.44	16443.36	11704.75
42	[81,81]	58774	116902.3	13197.39	6661.96	16048.58	11424.45
43	[86,84]	64725.4	128775.5	14526.12	7329.16	17667.27	12574.21
44	[89,87]	69386.2	138073.1	15566.91	7851.88	18935.1	13474.81
45	[90,93]	75022.3	149311.4	16826.64	8485.12	20469.17	14564.88
46	[94,97]	81740.7	162716.2	18326.36	9238.08	22296.25	15862.56
47	[98,100]	87865.8	174939.7	19693.12	9924.04	23961.55	17045.17
48	[101,104]	94190.9	187560.7	21104.87	10632.76	25681.52	18266.71
49	[105,108]	101701.3	202549.5	22780.59	11473.72	27723.32	19716.63
50	[112,109]	109493.7	218109.5	24517.34	12344.4	29840.23	21219.3
51	[116,113]	117580.1	234250.4	26321.06	13249.36	32038.19	22779.94
52	[120,117]	125954.5	250967.2	28188.78	14186.32	34314.23	24395.94
53	[115,115]	118634.4	236351.4	26557.01	13368.12	32325.4	22984.11
54	[121,126]	136799.5	272607.7	30609.39	15401.56	37263.28	26490.35
55	[127,131]	149298.8	297563.6	33396.01	16799	40659.52	28901.35
56	[138,132]	163479.4	325888.8	36554.64	18381.64	44510.27	31634.13
57	[145,139]	180906.6	360687.2	40439.15	20329.32	49244.86	34994.97
58	[146,156]	204481	407745	45697.44	22967.56	55652.43	39544.45
59	[157,167]	235430.6	469556.3	52593.67	26424.2	64058.74	45510.85
60	[178,168]	268538.2	535707.5	59964	30115.24	73045.63	51887.21
61	[180,179]	289369.1	577306.6	64606.5	32442.72	78704.31	55903.72
62	[182,182]	297497.6	593542.5	66417.32	33350.2	80911.79	57470.35
63	[181,195]	317030.2	632543	70771.83	35533.96	86218.9	61237.73
64	[200,196]	352123.2	702670.6	78582.22	39444.52	95743.09	67994.65

Table 4. Numerical representation of ISI , $ISI_{v\iota}$, R , $R_{v\iota}$, SCI ,and $SCI_{v\iota}$

To represent the correlation between the vicinal topological indices and the degree based topological indices the data in the above table are represented graphically using the method of least squares as shown in fig.2.





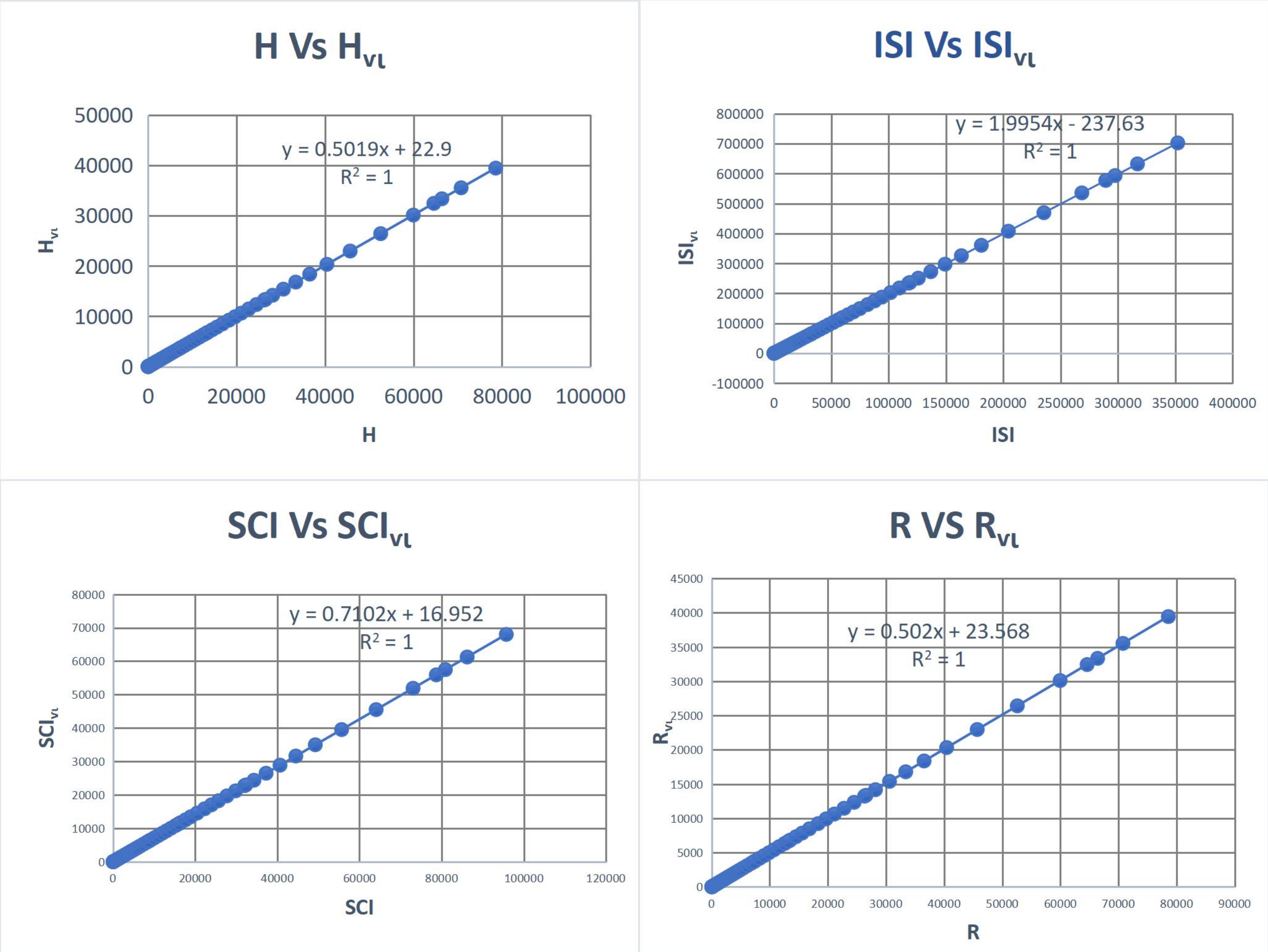


Figure 2. Correlation between the vicinal topological indices and degree based topological indices of $PTUZC_6[m,n]$.

4. R Code:

The R code to find geometric-arithmetic vicinal index, atom bond connectivity vicinal index, harmonic vicinal index, Inverse sum indeg vicinal index, Randić vicinal index, sum connectivity vicinal index where the output will be stored in the excel format by the name of "Topological_indices" after giving the input values of k (list of data required) and m, n

```
# Prompt the user to enter the number of values, convert it to an integer, and store it in 'k'

k=as.integer(readline(prompt="Enter the number of values  : "))

# Initialize two empty vectors 'a' and 'b' to store the values of 'm' and 'n' respectively

a=c()

b=c()

# Loop 'k' times to collect 'k' pairs of 'm' and 'n' values from the user

for (i in seq(1,k)){

  # Prompt the user to enter the value of 'm', convert it to an integer, and append it to vector 'a'

  p=as.integer(readline(prompt="Enter the values of m: "))

  if (p==1){

    print("Enter values of m greater than 1")

    break

  }

  a=append(a,p)

  # Prompt the user to enter the value of 'n', convert it to an integer, and append it to vector 'b'

  q=as.integer(readline(prompt="Enter the values of n: "))

  if (q==1){
```

```
    print("Enter values of n greater than 1")
    break
  }
  b=append(b,q)
}
# Define a function 'TP_' that calculates the six topological indices based on 'm' and 'n'
TP=function(m,n){
  GA_vicinal =(0.86*n)-(3*m)+(6*n*m)+(3.90)
  ABC_vicinal =(1.38*n)-(0.09*m)-(8.25)+(3.16*n*m)
  H_vicinal =(0.96*n)+(0.23*m)+(n*m)+(0.48)
  ISI_vicinal =(18*n*m)-(8.20*m)-(6.59*n)+(2.25)
  R_vicinal =(0.52)+(n*m)+(0.24*m)+(n)
  SCI_vicinal =(0.89*n)+(0.02*m)+(1.73*n*m)+(0.21)
  # Store the results in a list 'DL'
  DL=list(GA_vicinal,ABC_vicinal,H_vicinal,ISI_vicinal,R_vicinal,SCI_vicinal)
  # Return the list of topological indices
  return(DL)
}
# Call the 'TP' function with vectors 'a' and 'b', and store the results in 'Topology'
Topology=TP(a,b)
# Create a data frame 'DF' with six columns, each containing one of the topological indices
DF=data.frame(
  geometric_arithmetic_vicinal_index=Topology[[1]],
  atom_bond_connectivity_vicinal_index=Topology[[2]],
  harmonic_vicinal_index=Topology[[3]],
  inverse_sum_indeg_vicinal_index=Topology[[4]],
  randic_vicinal_index=Topology[[5]],
  sum_connectivity_vicinal_index=Topology[[6]]
)
# Write the data frame 'DF' to a CSV file named 'Topological_indices.csv'
write.csv(DF,"Topological_indices.csv")
```

5. Conclusion:

Vicinal degree and vicinal degree based topological indices are introduced in this study. By using mathematical derivation, edge partitions approach, and molecular graph analysis, we were able to compute generic formulae for geometric arithmetic vicinal index, atom bond connectivity vicinal index, harmonic vicinal index, inverse sum indeg vicinal index, Randić vicinal index, and sum connectivity vicinal index of planar polyhex zigzag nanotubes. A R code to compute the previously specified topological indices of $PTUZC_6[m,n]$ for any list of m,n has also been made available.

We tabulated the above vicinal based topological indices and geometric arithmetic index, atom bond connectivity index, harmonic index, inverse sum indeg index, Randić index, and sum connectivity index for 64 random values of m,n. Also, we obtained scattered plots representing the correlation between these above vicinal degree-based topological indices and degree based topological indices, by the method of least square. From the correlation we observed that vicinal topological indices and degree based topological indices mentioned above are highly correlated. Hence, we conclude that the vicinal topological indices are novel topological indices.

In the future, we intend to extend this article to analyze the chemical characteristics of planar polyhex zigzag nanotubes $\left(PTUZC_6[m,n]\right)$ using vicinal topological indices. Furthermore, we recommend investigating vicinal topological indices on diverse chemical compounds to determine their possible applicability.

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