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RESEARCH ARTICLE

Distance based Topological Indices of a Nanorod Graph

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ABSTRACT

In this article, we determine the distance-based topological indices such as Wiener index, Hyper Wiener index, Vertex Szeged index, Edge Szeged index, Edge-vertex Szeged index, Total Szeged index, and Padmakar-Ivan index of a Nanorod graph constructed from NaOH concentration. Additionally, we compare the numerical values of these distance-based topological indices with $k = 0.1, 0.09, 0.08, 0.07, 0.06, 0.05, 0.04, 0.03, 0.02$ *and* 0.01.

Keywords: Nanorod graph, Wiener index, Hyper Wiener index, Vertex Szeged index, Edge Szeged index, Edge-vertex Szeged index, Total Szeged index, Padmakar-Ivan index.

AMS Subject Classification: 05C90, 05C92

INTRODUCTION

For notation and graph theory terminology not provided here, we refer to [Gary Chartrand,2006]. In recent years, graph theory has generated significant interest in the field of mathematical chemistry, attracting mathematicians to formulate chemical structures and material properties. Chemical graph theory has numerous real-life applications and has gained popularity among researchers. A topological index is a numerical invariant of a molecular descriptor. It is also referred to as a graph-theoretic index, representing a numerical quantity associated with the molecular graph structure, which corresponds to unique chemical and physical properties. Topological indices can be categorized into different classes, including distance-based, degree-based, and eccentricity-based indices [Sowmya, 2020]. The Wiener index is the oldest topological index, which is the sum of distances between all pairs of vertices in a graph. This index was also shown by Harry Wiener to correlate well with various properties of alkanes in a series of research articles published from 1947 to 1948 [H.Wiener,1947 and Wiener H, 1948]. The Wiener index gained the great interestamidst of mathematicians around 1970 when it was introduced in graph theory under the name 'distance of a graph' [Plesnik J, 1984; L.Solts,1991;Entringer R.C.1976] and further studied in the form of the average distance of graphs [Chung F., 1988, Sanja S, 2018]. Some examples of distance-based topological indices include the Wiener index, Moster index, Edge Wiener index, and Szeged index, among others. In this study, we analyze distance-based topological indices for optical properties of a Nanorod graph. The authors Sonia et al. [Sonia, 2014] previously investigated the bioactivity of CuO Nanorods prepared under various concentrations of NaOH. The Nanorod graph was defined and generated by S. Sobiya, S. Sujitha, and M.K. Angel Jebitha using the methodology outlined in [Sonia, 2014], and various graphical parameters were studied in their previous work [S.Sobiya, 2023].

The distance is known as the shortest path and is denoted by $d(u,v)$ and the open neighborhood $N_{G_{Nr}}(v)$ is the set of vertices adjacent to v and an edge $e = uv \in E(G_{Nr})$.

$$N_u(e|G_{Nr}) = \{x \in V(G_{Nr}): d(u,x) < d(v,x)\}$$
$$M_u(e|G_{Nr}) = \{f \in E(G_{Nr}): d(u,f) < d(v,f)\}$$

The Cardinality of $N_u(e|G_{Nr})$ and $M_u(e|G_{Nr})$ is denoted by $n_u(e|G_{Nr})$ and $m_u(e|G_{Nr})$ respectively.[Micheal Arockiaraj,2019]

The Wiener index was introduced by Harry Wiener in 1947 and defined it as the sum of half of the distance between every pair of vertices in a graph.

(i.e) $W(G_{Nr}) = \frac{1}{2}\sum_{uv\in E(G_{Nr})} d(u,v)$

The Hyper Wiener index is

$$WW(G_{Nr}) = \frac{1}{2}\sum_{u,v\in E(G_{Nr})} [d(u,v) + (d(u,v))^2]$$

The Szeged index was introduced by Gutman in 1994 [I. Gutman,1994] and named as Gutman index. Later it is known as the Szeged index.

The Vertex Szeged index is

$$Sz_v(G_{Nr}) = \sum_{e\in E(G_{Nr})} n_u(e|G_{Nr}) n_v(e|G_{Nr})$$

The Edge Szeged index is

$$Sz_e(G_{Nr}) = \sum_{e\in E(G_{Nr})} m_u(e|G_{Nr}) m_v(e|G_{Nr})$$

The Edge-Vertex Szeged index is

$$Sz_{ev}(G_{Nr}) = \frac{1}{2}\sum_{e\in E(G_{Nr})} [n_u(e|G_{Nr}) m_v(e|G_{Nr}) + n_v(e|G_{Nr}) m_u(e|G_{Nr})$$

The Total Szeged index is

$$Sz_t(G_{Nr}) = Sz_v(G_{Nr}) + Sz_e(G_{Nr}) + 2Sz_{ev}(G_{Nr})$$

Padmakar V. Khadikar and Ivan Gutman [P.V.Khadikar,2000] introduced the Padmakar-Ivan index as,

$$PI(G_{Nr}) = \sum_{e\in E(G_{Nr})} [m_u(e|G_{Nr}) + m_v(e|G_{Nr})]$$

2 NANOROD GRAPH

The Nanorod graph, denoted asG_{Nr} is a simple connected graph with a vertex set $V(G) = \{v_1, v_2, v_3, \dots . v_n\}$ and an edge set $E(G)$ as defined in [S.Sobiya, 2023]. In $G_{Nr,}$the vertices correspond to different NaOH concentrations, and an edge exists between two vertices if they correspond to the UV spectrum parameters (pH, temperature, time, volume of solvent in a given ratio) associated with those NaOH concentrations. To construct the family of Nanorod graphs, various step values can be employed. In this article, we utilize ten step values denoted by 'k' (k = 0.1, 0.09, 0.08, 0.07, 0.06, 0.05, 0.04, 0.03, 0.02, and 0.01).The order of the Nanorod graph, represented as 'p,' is determined by $p = \left\lfloor\frac{1.5}{k} + 1\right\rfloor$, while the size is 'q,' and the reaction time is 't.' In our study, we set t = 2 hours and a pH value of 12 to calculate the topological indices. This article aims to determine various distance-based topological indices of the Nanorod graph G_{Nr}, considering its order (p), reaction time (t), and pH value.

Figure 1 shows a Nanorod graph with step value $k = 0.1$

3 THE DISTANCE BASED TOPOLOGICAL INDICES OF A NANOROD GRAPH

In this part, we will derive formulae for distance based topological indices , including the Wiener index, Hyper Wiener index, Edge-Vertex Szeged index, Edge Szeged index, Total Szeged index, and Padmakar-Ivan index, for a Nanorod graph.

Theorem 3.1 For a Nanorod graph G_{Nr}, the Wiener index is

$$W(G_{Nr}) = \begin{cases} \left[\frac{4.5p}{1.5} + \frac{p}{pH}n^3 - \frac{6p}{pH}n^2 + \frac{15p}{pH}n - \frac{8p}{pH}\right] + \frac{1}{2}size(q) if\ k = 0.1, n = t-1, k = 0.09, n = t, k = 0.08, \\ n = t+1\ and\ k = 0.07, k = t+2 \\ \left[\frac{p^2}{0.5pH} - \frac{2p}{pH}n^2 + \frac{15p}{pH}n - \frac{31p}{pH} + \frac{4.5p}{1.5}\right] + \frac{1}{2}size(q)\ if\ k = 0.06, n = t-1, k = 0.05, n = t\ and \\ k = 0.04, n = t+1 \\ \left[\frac{p^2}{0.5pH} + \frac{36.7p}{pH}n^2 - \frac{77.5p}{pH}n + \frac{57.2p}{pH} + \frac{4.5p}{1.5}\right] + \frac{1}{2}size(q)\ if\ k = 0.03, n = t-1, k = 0.02, n = t\ and \\ k = 0.01, n = t+1 \end{cases}$$

Proof. We know that the Wiener index of a Nanorod graph G_{Nr} is

$$W(G_{Nr}) = \frac{1}{2}\sum_{u,v \in V(G_{Nr})} d(u,v)$$

It can easily see that, the distance between any of any vertices of a Nanorod graph is either one or two

Case(i) $d(u,v) = 1\ for\ all\ u,v \in V(G_{Nr})$ and for all k

In this case, $W(G_{Nr}) = \frac{1}{2}\sum_{u,v \in V(G_{Nr})} d(u,v)$

$$= \frac{1}{2}[d(u_1,v_1) + \cdots . + d(u_2,v_2) + \cdots \ldots + d(u_n,v_n) + \cdots ..]$$

$$= \frac{1}{2}[1 + 1 + \cdots \ldots .]$$

$$= \frac{1}{2}size(q)$$

Case(ii) $d(u,v) = 2\ for\ all\ u,v \in V(G_{Nr})$ and for different k

Subcase a) When $k = 0.1, 0.09, 0.08, 0.07$

$$W(G_{Nr}) = \frac{1}{2}[d(u_1,v_2) + \cdots + d(u_2,v_3) + \cdots \ldots \ldots .]$$

$$= \frac{1}{2}[2 + 2 + 2 + \cdots \ldots]$$

$$= \frac{1}{2}[3p + \frac{p}{pH}(n^3 - 6n^2 - 15n - 8) + \frac{p}{1.5}]2$$

$$= [\frac{4.5p}{1.5} + \frac{p}{pH}n^3 - \frac{6p}{pH}n^2 + \frac{15p}{pH}n - \frac{8p}{pH}]$$

Subcase b) When $k = 0.06, 0.05, 0.04$

$$W(G_{Nr}) = \frac{1}{2}[d(u_1,v_2) + \cdots + d(u_2,v_3) + \cdots \ldots \ldots .]$$

$$= \frac{1}{2}[2 + 2 + 2 + \cdots \ldots]$$

$$= \frac{1}{2}[3p + [\frac{p}{pH}[\frac{p}{0.5} - (2n^2 - 15n - 31) + \frac{p}{1.5}]2$$

$$= [\frac{p^2}{0.5pH} - \frac{2p}{pH}n^2 + \frac{15p}{pH}n - \frac{31p}{pH} + \frac{4.5p}{1.5}]$$

Subcase c) When $k = 0.03, 0.02, 0.01$

$$W(G_{Nr}) = \frac{1}{2}[d(u_1,v_2) + \cdots + d(u_2,v_3) + \cdots \ldots \ldots .]$$

$$= \frac{1}{2}[2 + 2 + 2 + \cdots \ldots]$$

$= \frac{1}{2}[3p + [\frac{p}{pH}[\frac{p}{0.5} + (36.7n^2 - 77.5n + 57.2) + \frac{p}{1.5}]2$

$$= [\frac{p^2}{0.5pH} + \frac{36.7p}{pH}n^2 - \frac{77.5p}{pH}n + \frac{57.2p}{pH} + \frac{4.5p}{1.5}]$$

From Case(i) and Case(ii)

$\therefore W(G_{Nr})$for the Nanorod graph with step value $k = 0.1, 0.09, 0.08$ *and* 0.07

$$W(G_{Nr}) = \left[\frac{4.5p}{1.5} + \frac{p}{pH}n^3 - \frac{6p}{pH}n^2 + \frac{15p}{pH}n - \frac{8p}{pH}\right] + \frac{1}{2}size(q)$$

$\therefore W(G_{Nr})$for the Nanorod graph with step value $k = 0.06, 0.05, 0.04$

$$W(G_{Nr}) = \left[\frac{p^2}{0.5pH} - \frac{2p}{pH}n^2 + \frac{15p}{pH}n - \frac{31p}{pH} + \frac{4.5p}{1.5}\right] + \frac{1}{2}size(q)$$

$\therefore W(G_{Nr})$for the Nanorod graph with step value $k = 0.03, 0.02, 0.01$

$$W(G_{Nr}) = \left[\frac{p^2}{0.5pH} + \frac{36.7p}{pH}n^2 - \frac{77.5p}{pH}n + \frac{57.2p}{pH} + \frac{4.5p}{1.5}\right] + \frac{1}{2}size(q)$$

Theorem 3.2 LetG_{Nr} be a Nanorod graph. Then the Hyper Wiener index is

$$WW(G_{Nr}) = \begin{cases} p[\frac{p}{pH^2}(n^3 - 6n^2 + 15n - 8)^2 + \frac{22p}{(1.5)pH}(n^3 - 6n^2 + 15n - 8) + \frac{1}{pH}(n^3 - 6n^2 + 15n - 8) + \frac{90.75p}{3.375} \\ +3.6667 + \frac{size(q)(1 + size(q))}{2} \; if \; k = 0.1, n = t - 1, k = 0.09, n = t, k = 0.08, n = t + 1 \; and \\ k = 0.07, n = t + 2] \\ p[-\frac{4p^2}{(0.5)pH^2}(2n^2 - 15n + 31) + \frac{2p}{(pH)^2}(2n^2 - 15n + 31)^2 - \frac{22p}{(1.5)pH}(2n^2 - 15n + 31) - \\ \frac{1}{pH}(2n^2 - 15n + 31) + \frac{2p^3}{(0.25)(pH)^2} + \frac{11p^2}{(0.375)pH} + \frac{39p}{1.5} + \frac{p}{(0.5)pH} + 3.6667] + \frac{size(q)(1 + size(q))}{2} \\ if \; k = 0.06, n = t - 1, k = 0.05, n = t \; and \; k = 0.04, n = t + 1 \\ p[\frac{1346.89p}{pH^2}n^4 - \frac{5688.5p}{pH^2}n^3 + \frac{10204.73p}{pH^2} + \frac{73.4p^2}{(o.5)(pH)^2}n^2 - \frac{155p^2}{(0.5)(pH)^2}n + \frac{p^3}{(0.25)(pH)^2} + \frac{114.4p^2}{(0.5)(pH)^2} + \frac{3271.84p}{(pH)^2} \\ + \frac{330.3p}{(1.5)pH}n^2 + \frac{36.7}{pH}n^2 - \frac{697.5p}{(1.5)pH}n - \frac{77.5}{pH}n + \frac{9p^2}{(0.75)pH} + \frac{84.525p}{(0.75)pH} + \frac{20.25p}{2.25} + \frac{57.2}{pH} + 3] + \frac{size(q)(1 + size(q))}{2} \\ if \; k = 0.03, n = t - 1, k = 0.02, n = t \; and \; k = 0.01, n = t + 1 \end{cases}$$

Proof. We know that the Hyper Wiener index is

$$WW(G_{Nr}) = \frac{1}{2}\sum_{u,v \in E(G_{Nr})}[d(u,v) + (d(u,v))^2]$$

Since the distance between any pair of vertices of a Nanorod graph is either one or two, we have two cases.

Case(i) $d(u,v) = 1 \; for \; all \; u,v \in V(G_{Nr})$ and for all k

In this case, $WW(G_{Nr}) = \frac{1}{2}\sum_{uv \in V(G_{Nr})}\left[d(u,v) + \left(d(u,v)\right)^2\right]$

$$= \frac{1}{2}[[d(u_1,v_1) + \cdots . + d(u_2,v_2) + \cdots ... + d(u_n,v_n) + \cdots ..] + [d(u_1,v_1) + \cdots + d(u_2,v_2) + \cdots ... + d(u_n,v_n) + \cdots ..]^2]$$

$$= \frac{1}{2}[[1 + 1 + \cdots ....] + [1 + 1 + \cdots ...]^2]$$

$$= \frac{size(q)(1 + size(q))}{2}$$

Case(ii) $d(u,v) = 2 \; for \; all \; u,v \in V(G_{Nr})$ and for different k

Subcase a) When $k = 0.1, 0.09, 0.08, 0.07$

$$WW(G_{Nr}) = \frac{1}{2}\{[[d(u_1,v_2) + \cdots + d(u_2,v_3) + \cdots ... .] + [d(u_1,v_2) + \cdots + d(u_2,v_3) + \; ... ...]^2\}$$

$$= \frac{1}{2}\left\{\left[3p + \left(\frac{p}{pH}(n^3 - 6n^2 + 15n - 8) + \frac{p}{1.5}\right)\right]2 + \left[3p + \left(\frac{p}{pH}(n^3 - 6n^2 + 15n - \; 8) + \frac{p}{1.5}\right)\right]^2 4\right\}$$

$$= p[\frac{p}{pH^2}(n^3 - 6n^2 + 15n - 8)^2 + \frac{22p}{(1.5)pH}(n^3 - 6n^2 + 15n - 8) + \frac{1}{pH}(n^3 - 6n^2 + \; 15n - 8) + \frac{90.75p}{3.375} + 3.6667$$

Subcase b) When $k = 0.06, 0.05, 0.04$

$$WW(G_{Nr}) = \frac{1}{2}\{[d(u_1,v_2)+\cdots+d(u_2,v_3)+\cdots\ldots\ldots] + [d(u_1,v_2)+\cdots+d(u_2,v_3)+ \ldots\ldots\ldots]^2\}$$

$$= \frac{1}{2}\{\left[3p + \left(\frac{p}{pH}\left(\frac{p}{0.5} - (2n^2-15n+31)\right) + \frac{p}{1.5}\right)\right]2 + [3p + \left(\frac{p}{pH}\left(\frac{p}{0.5} - (2n^2-15n+31)\right) + \frac{p}{1.5}\right)]^2 4\}$$

$$= p[-\frac{4p^2}{(0.5)pH^2}(2n^2-15n+31) + \frac{2p}{(pH)^2}(2n^2-15n+31)^2 - \frac{22p}{(1.5)pH}(2n^2-15n+31) - \frac{1}{pH}(2n^2-15n+31) + \frac{2p^3}{(0.25)(pH)^2} + \frac{11p^2}{(0.375)pH} + \frac{39p}{1.5} + \frac{p}{(0.5)pH} + 3.6667]$$

Subcase c) When $k = 0.03, 0.02, 0.01$

$$WW(G_{Nr}) = \frac{1}{2}\{[d(u_1,v_2)+\cdots+d(u_2,v_3)+\cdots\ldots\ldots] + [d(u_1,v_2)+\cdots+d(u_2,v_3)+ \ldots\ldots\ldots]^2\}$$

$$= \frac{1}{2}\{\left[3p + \left(\frac{p}{pH}\left(\frac{p}{0.5} + (36.7n^2-77.5n+57.2)\right) + \frac{p}{1.5}\right)\right]2 + [3p + \left(\frac{p}{pH}\left(\frac{p}{0.5} + (36.7n^2-77.5n+57.2)\right) + \frac{p}{1.5}\right)]^2 4\}$$

$$= p[\frac{1346.89p}{pH^2}n^4 - \frac{5688.5p}{pH^2}n^3 + \frac{10204.73p}{pH^2} + \frac{73.4p^2}{(o.5)(pH)^2}n^2 - \frac{155p^2}{(0.5)(pH)^2}n + \frac{p^3}{(0.25)(pH)^2} + \frac{114.4p^2}{(0.5)(pH)^2} + \frac{3271.84p}{(pH)^2} + \frac{330.3p}{(1.5)pH}n^2 + \frac{36.7}{pH}n^2 - \frac{697.5p}{(1.5)pH}n - \frac{77.5}{pH}n + \frac{9p^2}{(0.75)pH} + \frac{84.525p}{(0.75)pH} + \frac{20.25p}{2.25} + \frac{57.2}{pH} + 3]$$

Therefore, from Case (i) and Case(ii)

$\therefore W(G_{Nr})$for the Nanorod graph with step value $k = 0.1, 0.09, 0.08\ and\ 0.07$

$$WW(G_{Nr}) = p[\frac{p}{pH^2}(n^3-6n^2+15n-8)^2 + \frac{22p}{(1.5)pH}(n^3-6n^2+15n-8) + \frac{1}{pH}(n^3-6n^2+15n-8) + \frac{90.75p}{3.375} + 3.6667 + \frac{size(q)(1+size(q))}{2}$$

$\therefore W(G_{Nr})$for the Nanorod graph with step value $k = 0.06, 0.05\ and\ 0.04$

$$WW(G_{Nr}) = p[-\frac{4p^2}{(0.5)pH^2}(2n^2-15n+31) + \frac{2p}{(pH)^2}(2n^2-15n+31)^2 - \frac{22p}{(1.5)pH}(2n^2-15n+31) - \frac{1}{pH}(2n^2-15n+31) + \frac{2p^3}{(0.25)(pH)^2} + \frac{11p^2}{(0.375)pH} + \frac{39p}{1.5} + \frac{p}{(0.5)pH} + 3.6667] + \frac{size(q)(1+size(q))}{2}$$

$\therefore W(G_{Nr})$for the Nanorod graph with step value $k = 0.03, 0.02\ and\ 0.01$

$$WW(G_{Nr}) = p[\frac{1346.89p}{pH^2}n^4 - \frac{5688.5p}{pH^2}n^3 + \frac{10204.73p}{pH^2} + \frac{73.4p^2}{(o.5)(pH)^2}n^2 - \frac{155p^2}{(0.5)(pH)^2}n + \frac{p^3}{(0.25)(pH)^2} + \frac{114.4p^2}{(0.5)(pH)^2} + \frac{3271.84p}{(pH)^2} + \frac{330.3p}{(1.5)pH}n^2 + \frac{36.7}{pH}n^2 - \frac{697.5p}{(1.5)pH}n - \frac{77.5}{pH}n + \frac{9p^2}{(0.75)pH} + \frac{84.525p}{(0.75)pH} + \frac{20.25p}{2.25} + \frac{57.2}{pH} + 3] + \frac{size(q)(1+size(q))}{2}$$

Theorem 3.3 For a Nanorodgraph G_{Nr}, the Edge-Szeged index is

$$Sz_e(G_{Nr}) = \begin{cases} \frac{21823}{36}n^6 - \frac{24325}{4}n^5 + \frac{2299543}{36}n^4 - \frac{378245}{2}n^3 + \frac{2585746}{9}n^2 - 215519n - \frac{157p}{3}n^5 + 537pn^4 \\ -\frac{9062p}{3}n^3 + 13420pn^2 - 24928pn + 14220p + 63135 - \frac{139}{6}n^3 2^{(2n-1)} + \frac{321}{2}n^2 2^{(2n-1)} \\ -\frac{949}{3}n 2^{(2n-1)} + (183)2^{(2n-1)} + (2n^2-4n+20)p2^{(2n-1)} + 8n^3p^2 + 64n^2p^2 - 80np^2 + 800p^2 \\ if\ k = 0.1, n = t-1, k = 0.09, n = t, k = 0.08, n = t+1\ and\ k = 0.07, n = t+2 \\ -\frac{237650}{9}n^6 + \frac{695945}{2}n^5 - \frac{16311671}{9}n^4 + \frac{14332214}{3}n^3 - \frac{60477935}{9}n^2 + \frac{28679549}{6}n \\ -1346634 + 5960pn^5 - 305533pn^4 + \frac{1101807p}{2}n^3 + \frac{365899p}{6}n^2 + \frac{1387142p}{3}n - 111181p \\ +650p^2n^4 - 2855p^2n^3 + 8737p^2n^2 - 12833p^2n + 12749p^2 \\ if\ k = 0.06, n = t-1, k = 0.05, n = t\ , k = 0.04, n = t+1\ and\ k = 0.03, n = t+2 \\ 2088627p^2n^2 - 96767pn^2 - 2100113p^2n + 298308pn - 140612p + 476956p^2 + 650n^2 - 3632n \\ +4920\ \ if\ k = 0.02, n = t-1\ and\ k = 0.01, n = t \end{cases}$$

Proof. We know that the Edge-Szeged index of a Nanorod graph is

$$Sz_e(G_{Nr}) = \sum_{e\in E(G_{Nr})} m_u(e|G_{Nr})m_v(e|G_{Nr})$$

Case(i) When $k = 0.1, 0.09, 0.08, 0.07$

$$m_u(e|G_{Nr}) = \left[-\frac{157}{6}n^3 + \frac{525}{2}n^2 - \frac{1744}{3}n + 345 + 2^{(2n-1)} + (4n+40)p\right]$$

$$m_v(e|G_{Nr}) = [-\frac{139}{6}n^3 + \frac{321}{2}n^2 - \frac{949}{3}n + 183 + (2n^2 - 4n + 20)p]$$

$$Sz_e(G_{Nr}) = m_1(e|G_{Nr})m_1(e|G_{Nr}) + m_2(e|G_{Nr})m_2(e|G_{Nr}) + \cdots \ldots ....$$

$$= \left[-\frac{157}{6}n^3 + \frac{525}{2}n^2 - \frac{1744}{3}n + 345 + 2^{(2n-1)} + (4n+40)p\right][-\frac{139}{6}n^3 + \frac{321}{2}n^2 - \frac{949}{3}n + 183 + (2n^2 - 4n + 20)p]$$

$$= \frac{21823}{36}n^6 - \frac{24325}{4}n^5 + \frac{2299543}{36}n^4 - \frac{378245}{2}n^3 + \frac{2585746}{9}n^2 - 215519n - \frac{157p}{3}n^5 + 537pn^4 - \frac{9062p}{3}n^3 + 13420pn^2 - 24928pn + 14220p + 63135 - \frac{139}{6}n^3 2^{(2n-1)} + \frac{321}{2}n^2 2^{(2n-1)} - \frac{949}{3}n 2^{(2n-1)} + (183)2^{(2n-1)} + (2n^2 - 4n + 20)p2^{(2n-1)} + 8n^3p^2 + 64n^2p^2 - 80np^2 + 800p^2$$

Case(ii) When $k = 0.06, 0.05, 0.04, 0.03$

$$m_u(e|G_{Nr}) = \left[-\frac{490}{3}n^3 + \frac{2363}{2}n^2 - \frac{14515}{6}n + 1422 + (50n^2 - 135n + 209)p\right]$$

$$m_v(e|G_{Nr}) = [\frac{485}{3}n^3 - 961n^2 + \frac{5251}{3}n - 947 + (13n^2 - 22n + 61)p]$$

$$Sz_e(G_{Nr}) = m_1(e|G_{Nr})m_1(e|G_{Nr}) + m_2(e|G_{Nr})m_2(e|G_{Nr}) + \cdots \ldots ....$$

$$= \left[-\frac{490}{3}n^3 + \frac{2363}{2}n^2 - \frac{14515}{6}n + 1422 + (50n^2 - 135n + 209)p\right][\frac{485}{3}n^3 - 961n^2 + \frac{5251}{3}n - 947 + (13n^2 - 22n + 61)p]$$

$$= -\frac{237650}{9}n^6 + \frac{695945}{2}n^5 - \frac{16311671}{9}n^4 + \frac{14332214}{3}n^3 - \frac{60477935}{9}n^2 + \frac{28679549}{6}n - 1346634 + 5960pn^5 - 305533pn^4 + \frac{1101807p}{2}n^3 + \frac{365899p}{6}n^2 + \frac{1387142p}{3}n - 111181p + 650p^2n^4 - 2855p^2n^3 + 8737p^2n^2 - 12833p^2n + 12749p^2$$

Case(iii) When $k = 0.02, 0.01$

$$m_u(e|G_{Nr}) = [-25n + 82 + (3067n - 2021)p]$$

$$m_v(e|G_{Nr}) = [-26n + 60 + (681n - 236)p]$$

$$Sz_e(G_{Nr}) = m_1(e|G_{Nr})m_1(e|G_{Nr}) + m_2(e|G_{Nr})m_2(e|G_{Nr}) + \cdots \ldots ....$$

$$= [-25n + 82 + (3067n - 2021)p][-26n + 60 + (681n - 236)p]$$

$$= 2088627p^2n^2 - 96767pn^2 - 2100113p^2n + 298308pn - 140612p + 476956p\text{^}2 + 650n\text{^}2 - 3632n + 4920$$

Theorem 3.4 Let G_{Nr} be a Nanorod graph. Then the Edge-vertex Szeged index is

$$Sz_{ev}(G_{Nr}) = \begin{cases} \frac{1}{2}[\frac{695}{36}n^6 - \frac{893}{2}n^5 + \frac{118907}{36}n^4 - \frac{67537}{6}n^3 + \frac{357169}{18}n^2 - \frac{52945}{3}n + 6222 - \frac{149p}{6}n^5 + 1284pn^4 - 1431pn^3 \\ +1630pn^2 - \frac{7013p}{3}n + 1412p + 2p^2n^4 - 6p^2n^3 + 32p^2n^2 - 36p^2n + 80p^2] \\ \text{if } k = 0.1, n = t-1, k = 0.09, n = t, k = 0.08, n = t+1 \text{ and } k = 0.07, n = t+2 \\ \frac{1}{2}[\frac{631955}{18}n^6 - \frac{2509303}{6}n^5 + \frac{36159386}{9}n^4 - \frac{29767028}{3}n^3 + \frac{119118809}{18}n^2 - \frac{9009719}{2}n + 1222577 + \frac{23729p}{6}n^5 \\ -29161pn^4 + \frac{574684p}{3}n^3 - 1199376pn^2 + \frac{488541p}{2}n - 114737p + 91p^2n^4 - 219p^2n^3 + 1031p^2n^2 \\ -1141p^2n + 2318p^2] \text{ if } k = 0.06, n = t-1, k = 0.05, n = t, k = 0.04, n = t+1 \text{ and } \\ k = 0.03, n = t+2 \\ \frac{1}{2}[-1118n^2 + 1930n + 1500 + 2087pn^2 + 88019pn - 48320p + 712326p^2n^2 - 728323p^2n \\ +166852p^2] \text{ if } k = 0.02, n = t-1 \text{ and } k = 0.01, n = t \end{cases}$$

Proof. We know that the Edge-Vertex Szeged index of a Nanorod graph is

$Sz_{ev}(G_{Nr}) = \frac{1}{2}\sum_{e\in E(G_{Nr})}[n_u(e|G_{Nr})m_v(e|G_{Nr}) + n_v(e|G_{Nr})m_u(e|G_{Nr})]$

Case(i) When $k = 0.1, 0.09, 0.08, 0.07$

$$n_u(e|G_{Nr}) = -\frac{5}{6}n^3 + \frac{27}{2}n^2 - \frac{113}{3}n + 34 + (n^2 - n + 4)p$$
$$n_v(e|G_{Nr}) = 0$$
$$m_u(e|G_{Nr}) = -\frac{157}{6}n^3 + \frac{525}{2}n^2 - \frac{1744}{3}n + 345 + 2^{(2n-1)} + (4n + 40)p$$
$$m_v(e|G_{Nr}) = -\frac{139}{6}n^3 + \frac{321}{2}n^2 - \frac{949}{3}n + 183 + (2n^2 - 4n + 20)p$$
$$Sz_{ev}(G_{Nr}) = \frac{1}{2}\Big[\Big(-\frac{5}{6}n^3 + \frac{27}{2}n^2 - \frac{113}{3}n + 34 + (n^2 - n + 4)p\Big)\Big(m_v(e|G_{Nr}) = -\frac{139}{6}n^3 + \frac{321}{2}n^2 - \frac{949}{3}n + 183 + (2n^2 - 4n + 20)p\Big)\Big] + [(0)(-\frac{157}{6}n^3 + \frac{525}{2}n^2 - \frac{1744}{3}n + 345 + 2^{(2n-1)} + (4n + 40)p)]$$
$$= \frac{1}{2}[\frac{695}{36}n^6 - \frac{893}{2}n^5 + \frac{118907}{36}n^4 - \frac{67537}{6}n^3 + \frac{357169}{18}n^2 - \frac{52945}{3}n + 6222 - \frac{149p}{6}n^5 + 1284pn^4 - 1431pn^3 + 1630pn^2 - \frac{7013p}{3}n + 1412p + 2p^2n^4 - 6p^2n^3 + 32p^2n^2 - 36p^2n + 80p^2]$$

Case(ii) When $k = 0.06, 0.05, 0.04, 0.03$

$$n_u(e|G_{Nr}) = \frac{1303}{6}n^3 - \frac{2592}{2}n^2 + \frac{14225}{6}n - 1291 + (7n^2 - 5n + 38)p$$
$$n_v(e|G_{Nr}) = 0$$
$$m_u(e|G_{Nr}) = -\frac{490}{3}n^3 + \frac{2363}{2}n^2 - \frac{14515}{6}n + 1422 + (50n^2 - 135n + 209)p$$
$$m_v(e|G_{Nr}) = \frac{485}{3}n^3 - 961n^2 + \frac{5251}{3}n - 947 + (13n^2 - 22n + 61)p$$
$$Sz_{ev}(G_{Nr}) = \frac{1}{2}[\Big(\frac{1303}{6}n^3 - \frac{2592}{2}n^2 + \frac{14225}{6}n - 1291 + (7n^2 - 5n + 38)p\Big)\Big(\frac{485}{3}n^3 - 961n^2 + \frac{5251}{3}n - 947 + (13n^2 - 22n + 61)p\Big) + (0)(-\frac{490}{3}n^3 + \frac{2363}{2}n^2 - \frac{14515}{6}n + 1422 + (50n^2 - 135n + 209)p)]$$
$$= \frac{1}{2}[\frac{631955}{18}n^6 - \frac{2509303}{6}n^5 + \frac{36159386}{9}n^4 - \frac{29767028}{3}n^3 + \frac{119118809}{18}n^2 - \frac{9009719}{2}n + 1222577 + \frac{23729p}{6}n^5 - 29161pn^4 + \frac{574684p}{3}n^3 - 1199376pn^2 + \frac{488541p}{2}n - 114737p + 91p^2n^4 - 219p^2n^3 + 1031p^2n^2 - 1141p^2n + 2318p^2]$$

Case(iii) When $k = 0.02, 0.01$

$$n_u(e|G_{Nr}) = 43n + 25 + (1046n - 707)p$$
$$n_v(e|G_{Nr}) = 0$$
$$m_u(e|G_{Nr}) = -25n + 82 + (3067n - 2021)p$$
$$m_v(e|G_{Nr}) = -26n + 60 + (681n - 236)p$$
$$Sz_{ev}(G_{Nr}) = \frac{1}{2}[(43n + 25 + (1046n - 707)p)(-26n + 60 + (681n - 236)p) + (0)(-25n + 82 + (3067n - 2021)p)]$$
$$= \frac{1}{2}[-1118n^2 + 1930n + 1500 + 2087pn^2 + 88019pn - 48320p + 712326p^2n^2 - 728323p^2n + 166852p^2]$$

Theorem 3.5 If G_{Nr} be a Nanorod graph, then the Total Szeged index is

$$Sz_t(G_{Nr}) = \begin{cases} \frac{1251}{2}n^6 - \frac{26111}{4}n^5 + \frac{403075}{6}n^4 - \frac{601136}{3}n^3 + \frac{1842887}{6}n^2 - \frac{699502}{3}n - \frac{463}{6}pn^5 + 1821pn^4 \\ -\frac{13355p}{3}n^3 + 15050pn^2 - \frac{81788}{3}pn + 15632p + 69357 + 2p^2n^4 + 2p^2n^3 + 96p^2n^2 \\ -116p^2n + 880p^2 - \frac{139}{6}n^3 2^{(2n-1)} + \frac{321}{2}n^2 2^{(2n-1)} - \frac{949}{3}n2^{(2n-1)} + 1832^{(2n-1)} \\ +(2n^2-4n+20)p2^{(2n-1)}\ if\ k=0.1, n=t-1, k=0.09, n=t, k=0.08, n=t+1\ and \\ k=0.07, k=t+2 \\ \frac{156655}{18}n^6 - \frac{210734}{3}n^5 + \frac{6615905}{3}n^4 - 5144938n^3 - \frac{1837061}{18}n^2 + \frac{825196}{3}n - 124057 \\ +\frac{59489}{6}pn^5 - 334694pn^4 + \frac{4454789}{6}pn^3 - \frac{6830357p}{6}n^2 + \frac{4239907p}{6}n - 225918p \\ +741p^2n^4 - 3074p^2n^3 + 9768p^2n^2 - 13974p^2n + 15067p^2 \\ if\ k=0.06, n=t-1, k=0.05, n=t, k=0.04, n=t+1\ and\ k=0.03, n=t+2 \\ 532n^2 - 1702n + 6420 - 94680pn^2 + 386327pn - 188932p + 2800953p^2n^2 \\ -2828436p^2n + 643808p^2\ \ if\ k=0.02, n=t-1\ and\ k=0.01, n=t \end{cases}$$

Proof. We know that the Total Szeged index of a Nanorod graph is

$$Sz_t(G_{Nr}) = Sz_v(G_{Nr}) + Sz_e(G_{Nr}) + 2Sz_{ev}(G_{Nr})$$

Case(i) When $k = 0.1, k = 0.09, k = 0.08, k = 0.07$

$$Sz_v(G_{Nr}) = 0$$

$$Sz_e(G_{Nr}) = \frac{21823}{36}n^6 - \frac{24325}{4}n^5 + \frac{2299543}{36}n^4 - \frac{378245}{2}n^3 + \frac{2585746}{9}n^2 - 215519n - \frac{157p}{3}n^5 + 537pn^4$$
$$-\frac{9062p}{3}n^3 + 13420pn^2 - 24928pn + 14220p + 63135 - \frac{139}{6}n^3 2^{(2n-1)} + \frac{321}{2}n^2 2^{(2n-1)}$$
$$-\frac{949}{3}n2^{(2n-1)} + (183)2^{(2n-1)} + (2n^2-4n+20)p2^{(2n-1)} + 8n^3p^2 + 64n^2p^2 - 80np^2 + 800p^2$$

$$Sz_{ev}(G_{Nr}) = \frac{1}{2}\Big[\frac{695}{36}n^6 - \frac{893}{2}n^5 + \frac{118907}{36}n^4 - \frac{67537}{6}n^3 + \frac{357169}{18}n^2 - \frac{52945}{3}n + 6222 - \frac{149p}{6}n^5$$
$$+ 1284pn^4 - 1431pn^3 + 1630pn^2 - \frac{7013p}{3}n + 1412p + 2p^2n^4 - 6p^2n^3 + 32p^2n^2$$
$$- 36p^2n + 80p^2\Big]$$

$$Sz_t(G_{Nr}) = 0 + \frac{21823}{36}n^6 - \frac{24325}{4}n^5 + \frac{2299543}{36}n^4 - \frac{378245}{2}n^3 + \frac{2585746}{9}n^2 - 215519n - \frac{157p}{3}n^5 + 537pn^4$$
$$-\frac{9062p}{3}n^3 + 13420pn^2 - 24928pn + 14220p + 63135 - \frac{139}{6}n^3 2^{(2n-1)} + \frac{321}{2}n^2 2^{(2n-1)}$$
$$-\frac{949}{3}n2^{(2n-1)} + (183)2^{(2n-1)} + (2n^2-4n+20)p2^{(2n-1)} + 8n^3p^2 + 64n^2p^2 - 80np^2 + 800p^2$$
$$+ 2\Big[\frac{1}{2}\Big[\frac{695}{36}n^6 - \frac{893}{2}n^5 + \frac{118907}{36}n^4 - \frac{67537}{6}n^3 + \frac{357169}{18}n^2 - \frac{52945}{3}n + 6222 - \frac{149p}{6}n^5$$
$$+ 1284pn^4 - 1431pn^3 + 1630pn^2 - \frac{7013p}{3}n + 1412p + 2p^2n^4 - 6p^2n^3 + 32p^2n^2 - 36p^2n + 80p^2\Big]\Big]$$

$$= \frac{1251}{2}n^6 - \frac{26111}{4}n^5 + \frac{403075}{6}n^4 - \frac{601136}{3}n^3 + \frac{1842887}{6}n^2 - \frac{699502}{3}n - \frac{463}{6}pn^5 + 1821pn^4$$
$$-\frac{13355p}{3}n^3 + 15050pn^2 - \frac{81788}{3}pn + 15632p + 69357 + 2p^2n^4 + 2p^2n^3 + 96p^2n^2$$
$$- 116p^2n + 880p^2 - \frac{139}{6}n^3 2^{(2n-1)} + \frac{321}{2}n^2 2^{(2n-1)} - \frac{949}{3}n2^{(2n-1)} + 1832^{(2n-1)}$$
$$+ (2n^2-4n+20)p2^{(2n-1)}$$

Case(ii) When $k = 0.06, k = 0.05, k = 0.04, k = 0.03$

$$Sz_v(G_{Nr}) = 0$$

$$Sz_e(G_{Nr}) = -\frac{237650}{9}n^6 + \frac{695945}{2}n^5 - \frac{16311671}{9}n^4 + \frac{14332214}{3}n^3 - \frac{60477935}{9}n^2 + \frac{28679549}{6}n - 1346634$$
$$+ 5960pn^5 - 305533pn^4 + \frac{1101807p}{2}n^3 + \frac{365899p}{6}n^2 + \frac{1387142p}{3}n - 111181p + 650p^2n^4$$
$$- 2855p^2n^3 + 8737p^2n^2 - 12833p^2n + 12749p^2$$

$$Sz_{ev}(G_{Nr}) = \frac{1}{2}[\frac{631955}{18}n^6 - \frac{2509303}{6}n^5 + \frac{36159386}{9}n^4 - \frac{29767028}{3}n^3 + \frac{119118809}{18}n^2 - \frac{9009719}{2}n + 1222577 + \frac{23729p}{6}n^5 - 29161pn^4 + \frac{574684p}{3}n^3 - 1199376pn^2 + \frac{488541p}{2}n - 114737p + 91p^2n^4 - 219p^2n^3 + 1031p^2n^2 - 1141p^2n + 2318p^2]$$

$$Sz_t(G_{Nr}) = 0 + -\frac{237650}{9}n^6 + \frac{695945}{2}n^5 - \frac{16311671}{9}n^4 + \frac{14332214}{3}n^3 - \frac{60477935}{9}n^2 + \frac{28679549}{6}n - 1346634 + 5960pn^5 - 305533pn^4 + \frac{1101807p}{2}n^3 + \frac{365899p}{6}n^2 + \frac{1387142p}{3}n - 111181p + 650p^2n^4 - 2855p^2n^3 + 8737p^2n^2 - 12833p^2n + 12749p^2 + 2[\frac{1}{2}[\frac{631955}{18}n^6 - \frac{2509303}{6}n^5 + \frac{36159386}{9}n^4 - \frac{29767028}{3}n^3 + \frac{119118809}{18}n^2 - \frac{9009719}{2}n + 1222577 + \frac{23729p}{6}n^5 - 29161pn^4 + \frac{574684p}{3}n^3 - 1199376pn^2 + \frac{488541p}{2}n - 114737p + 91p^2n^4 - 219p^2n^3 + 1031p^2n^2 - 1141p^2n + 2318p^2]]$$

$$Sz_t(G_{Nr}) = \frac{156655}{18}n^6 - \frac{210734}{3}n^5 + \frac{6615905}{3}n^4 - 5144938n^3 - \frac{1837061}{18}n^2 + \frac{825196}{3}n - 124057 + \frac{59489}{6}pn^5 - 334694pn^4 + \frac{4454789}{6}pn^3 - \frac{6830357p}{6}n^2 + \frac{4239907p}{6}n - 225918p + 741p^2n^4 - 3074p^2n^3 + 9768p^2n^2 - 13974p^2n + 15067p^2$$

Case(iii) When $k = 0.02, k = 0.01$

$$Sz_v(G_{Nr}) = 0$$

$$Sz_e(G_{Nr}) = 2088627p^2n^2 - 96767pn^2 - 2100113p^2n + 298308pn - 140612p + 476956p\text{^}2 + 650n\text{^}2 - 3632n + 4920$$

$$Sz_{ev}(G_{Nr}) = \frac{1}{2}[-1118n^2 + 1930n + 1500 + 2087pn^2 + 88019pn - 48320p + 712326p^2n^2 - 728323p^2n + 166852p^2]$$

$$Sz_t(G_{Nr}) = 0 + 2088627p^2n^2 - 96767pn^2 - 2100113p^2n + 298308pn - 140612p + 476956p^2 + 650n^2 - 3632n + 4920 + 2[\frac{1}{2}[-1118n^2 + 1930n + 1500 + 2087pn^2 + 88019pn - 48320p + 712326p^2n^2 - 728323p^2n + 166852p^2]]$$

Theorem 3.6 For a Nanorodgraph G_{Nr}, the Padmakar-Ivan index is

$$PI(G_{Nr}) = \begin{cases} -\frac{148}{3}n^3 + 423n^2 - \frac{2693}{3}n + 528 + 2^{(2n-1)} + 2pn^2 + 60p \\ if\ k = 0.1, n = t-1, k = 0.09, n = t, k = 0.08, n = t+1\ and\ k = 0.07, n = t+2 \\ -\frac{5}{3}n^3 + 441n^2 - \frac{4013}{3}n + 475 + 63pn^2 - 157pn + 270p \\ if\ k = 0.06, n = t-1, k = 0.05, n = t, k = 0.04, n = t+1\ and\ k = 0.03, n = t+2 \\ -51n + 142 + 3748pn - 2257p \quad if\ k = 0.02, n = t-1\ and\ k = 0.01, n = t \end{cases}$$

Proof. We know that the Padmakar -Ivan index of a Nanorod Graph is

$$PI(G_{Nr}) = \sum_{e \in E(G_{Nr})} [m_u(e|G_{Nr}) + m_v(e|G_{Nr})]$$

Case(i) When $k = 0.1, 0.09, 0.08, 0.07$

$$m_u(e|G_{Nr}) = -\frac{157}{6}n^3 + \frac{525}{2}n^2 - \frac{1744}{3}n + 345 + 2^{(2n-1)} + (4n+40)p$$

$$m_v(e|G_{Nr}) = -\frac{139}{6}n^3 + \frac{321}{2}n^2 - \frac{949}{3}n + 183 + (2n^2 - 4n + 20)p$$

$$PI(G_{Nr}) = -\frac{157}{6}n^3 + \frac{525}{2}n^2 - \frac{1744}{3}n + 345 + 2^{(2n-1)} + (4n+40)p + -\frac{139}{6}n^3 + \frac{321}{2}n^2 - \frac{949}{3}n + 183 + (2n^2 - 4n + 20)p$$

$$= -\frac{148}{3}n^3 + 423n^2 - \frac{2693}{3}n + 528 + 2^{(2n-1)} + 2pn^2 + 60p$$

Case(ii) When $k = 0.06, 0.05, 0.04, 0.03$

$$m_u(e|G_{Nr}) = -\frac{490}{3}n^3 + \frac{2363}{2}n^2 - \frac{14515}{6}n + 1422 + (50n^2 - 135n + 209)p$$

$$m_v(e|G_{Nr}) = \frac{485}{3}n^3 - 961n^2 + \frac{5251}{3}n - 947 + (13n^2 - 22n + 61)p$$

$$PI(G_{Nr}) = -\frac{490}{3}n^3 + \frac{2363}{2}n^2 - \frac{14515}{6}n + 1422 + (50n^2 - 135n + 209)p + \frac{485}{3}n^3 - 961n^2 + \frac{5251}{3}n - 947 + (13n^2 - 22n + 61)p$$

$$= -\frac{5}{3}n^3 + 441n^2 - \frac{4013}{3}n + 475 + 63pn^2 - 157pn + 270p$$

Case(iii) When $k = 0.02, 0.01$

$$m_u(e|G_{Nr}) = -25n + 82 + (3067n - 2021)p$$

$$m_v(e|G_{Nr}) = -26n + 60 + (681n - 236)p$$

$$PI(G_{Nr}) = -25n + 82 + (3067n - 2021)p + -26n + 60 + (681n - 236)p$$

$$= -51n + 142 + 3748pn - 2257p$$

OBSERVATION 3.7

For the Vertex Szeged index, we take any pair of vertices $u, v \in G_{Nr}$ and find the distance of $d(u,x)$ and $d(v,x)$ and then verify whether $d(u,x) < d(v,x)$and $d(v,x) < d(u,x)$. But in the Nanorod graph, we can observe that, $d(u,x) < d(v,x)$ *and* $d(v,x) \geq d(u,x)$. Since the condition $d(v,x) < d(u,x)$ is not satisfied for the Nanorod graph, the Vertex Szeged index is zero.

The table below displays numerical values of distance-based topological indices, including the Wiener index, Hyper Wiener index, Vertex Szeged index, Edge Szeged index, Edge-Vertex Szeged index, Total Szeged index, and Padmakar-Ivan index, for various step values of k: 0.1, 0.09, 0.08, 0.07, 0.06, 0.05, 0.04, 0.03, 0.02, and 0.01.

Step value k	$W(G_{Nr})$	$WW(G_{Nr})$	$Sz_e(G_{Nr})$	$Sz_{ev}(G_{Nr})$	$Sz_t(G_{Nr})$	$PI(G_{Nr})$
0.1	80.1667	9347.7778	210351.75	13494	211163.75	998
0.09	92.5	12244.3055	428301	115604	−319129.667	1194
0.08	115.8333	18196.3056	1684050.25	697274.25	3176945.75	1824
0.07	158.1667	47820.4444	5855509.67	2667613	10905090.3	−2660
0.06	229.6667	68936.1111	21610278.7	−12518451.6	−3426624.56	4152.6667
0.05	313.1667	147771.375	34203854	−52001264.5	−71010645.9	6060.3333
0.04	462.1667	323236.333	−208527539	−100360911.5	−571577797	24834
0.03	948.7	712407.39	$-1.51900794e9$	−112150783	$-6.87964558e9$	100223.667
0.02	2144	3681383.22	$2.69318726e9$	437258264	$3.56770479e9$	113407
0.01	8715.0833	−342714246	$1.05607267e11$	$1.39850748e9$	$1.41186206e11$	791129

From the table above, we can easily observe that the Wiener index produces only positive values. Furthermore, it is evident that as the number of vertices in a Nanorod graph increases, the corresponding numerical values of the Wiener index also increase. Therefore, our study confirms that the Wiener index is the most suitable index among all distance-based topological indices.

CONCLUSION

In this article, we determined the general formula for certain distance-based topological indices and compared their exact values with step values of k: 0.1, 0.09, 0.08, 0.07, 0.06, 0.05, 0.04, 0.03, 0.02, and 0.01.

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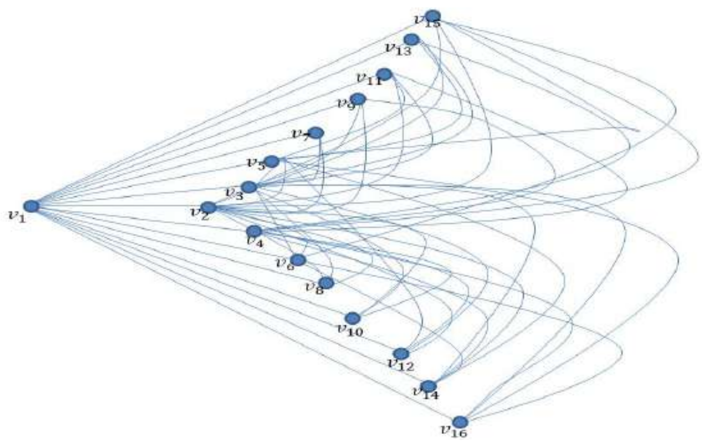

Figure 1 :Nanorod graph G_{Nr} with $k = 0.1$