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Research Article

On Neighborhood Degree-Based Topological Analysis of Polyphenylene Network

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Organic compounds such as polyphenylene are very important and useful for the synthesis of many new organic compounds due to their physio-chemical properties. To ascertain these properties, one can use QSPR/QSAR methods which necessitate the computation of topological indices. The topological indices based on two newly introduced abstract notions of ev-degree and ve-degree are in practice to model numerous chemical properties as well as physical properties of organic, inorganic, hybrid, and biological compounds. In this study, we computed a certain number of topological indices for the chemical graph of polyphenylene network which will help to model some of its physio-chemical properties.

1. Introduction

The detailed critical inspection in order to discover essential features or meanings of chemical compounds graphically is known as chemical graph theory. It is the branch of mathematics, which alloys chemistry and graph theory. In graph theory, a simple graph or just graph $G(V, E)$ is constructed by two sets: $V = \{v_1, \ldots, v_n\}$, the set of vertices, and $E = \{e_1, \ldots, e_m\}$, the set of edges. Each $v \in V$ represents a node in the graph and each $e \in E$ denotes the line joining two nodes.

In chemical graph theory, the image obtained from diffraction of X-rays or electron microscopy of a compound (biological or chemical) is drawn into plane and lighted upon its symmetry, and then, peculiarities of this compound is mathematically modeled. The simple sketch of the image of compound is known as the chemical graph where we assume that the ends or vertices are atoms and lines or edges are the bonds between the atoms. Chemical graph theory helps to understand different properties, namely, molecular structure, kinetics of molecules, atoms or electrons, chain or patterns of polymers, crystals and clusters, aromaticity, nuclear magnetic resonance (NMR) analysis, depicting orbitals, and electrons behaviors. Ante Graovac, Alexandru Balaban, Haruo Hosoya, Iv a n Gutman, Nenad Trinajstic, and Milan Randic are few scientists who introduced graph theory in chemistry [1].

The job of mathematical modeling the properties of chemical compounds is done by topological indices which we define as *a number obtained by a real-valued function,* $g = g(e), g = g(v) \text{or} g = g(e, v)$, *that is applied to any chemical graph (or molecular structure) of a compound to determine its topology, is known as topological graph index or just topological index (plural: topological indices), where* e and $v \in \mathbb{Z}^+$ *are edges and vertices of graph,* for example, Zagreb indices and their variants, distance indices, detour index, and Wiener index. There are different kinds of topological indices based on degree, distance, and counting [2]. Many physical and chemical properties of different chemical and biological compounds have been modeled mathematically by the aid of topological indices such as boiling point, anti-leishmanial effect, acute toxicity, radial scavenging activity, and many more [3–5]. In this study, we considered some topological indices based on degree of vertices and edges, ve-degree of vertices, and ev-degree of edges. To understand the terms used in formulas of topological indices, first, we consider the following basic definitions [6–8].

For a graph $X(V,E)$, we have

(1) Degree of a vertex v means the number of edges connected to the vertex v denoted by $\mathrm{d}_X(v)$

(2) The number $\mathrm{d}_X(v)+\mathrm{d}_X(w)-2$ is called *degree of edge e* if e is formed by joining the vertex v and w, denoted by $\mathrm{d}_X(e)$

(3) The set $N(w)=\{v\in V\colon v \text{ and } w \text{ are nodes of some edge } e\in E\}$ is called the *open neighborhood* of the vertex w

(4) The set $\{w\}\cup N(w)$ is the *closed neighborhood* of w denoted by $N[w]$

(5) The number of nonidentical edges that are incident to each vertex in the closed neighbourhood of the vertex v is the ve-degree of vertex v denoted by $d_X^{ve}v$ [9]

(6) If v and w are nodes of an edge e, then the order of $N[v]\cup N[w]$ is equal to the *ev-degree* [9] of edge e, denoted by $d_X^{ev}(e)$

For a graph $X(V,E)$, the topological indices under consideration are given below:

(i) Randić index [10]:

$$R(X)=\sum_{e=1}^{|E|}\frac{1}{\sqrt{d_X(u)\times d_X(v)}}. \tag{1}$$

(ii) *ev*-degree Randić index [11]:

$$R^{ev}(X)=\sum_{e=1}^{|E|}\frac{1}{\sqrt{d_X^{ev}(e)}}. \tag{2}$$

(iii) *ve*-degree Randić index:

$$R^{ve}(X)=\sum_{e=1}^{|E|}\frac{1}{\sqrt{d_X^{ve}(u)\times d_X^{ve}(v)}}. \tag{3}$$

(iv) Reciprocal *ve*-degree Randić index [12]:

$$RR^{ev}(H)=\sum_{e=1}^{|E|}d_X^{ev}(e)^{1/2}. \tag{4}$$

Milan Randić, a chemist, introduced the "branching index" in 1975 as a topological index R for evaluating the degree of branching in the carbon-atom skeleton of saturated hydrocarbons [10]. Moreover, it is also used to model the cavity surface area of different alcohols. In [11], Suleyman Ediz introduced *ev*–degree Randić (2) index and proved that it gives more accurate correlation than the previous one.

First ve-degree Zagreb beta index:

$$M_i^{\mathrm{bve}}(X)=\sum_{e=1}^{|E|}\left(d_X^{ve}v+d_X^{ve}w\right). \tag{5}$$

Second ve-degree Zagreb index:

$$M_{ii}^{ve}(X)=\sum_{e=1}^{|E|}\left(d_X^{ve}v\times d_X^{ve}w\right). \tag{6}$$

Redefined third ve-degree Zagreb index [13]:

$$\mathrm{RZG}_{iii}^{ve}(H)=\sum_{e=1}^{|E|}\left(d_X^{ve}(u)\times d_X^{ve}(v)\right)\left(d_X^{ve}(u)+d_X^{ve}(v)\right). \tag{7}$$

The modified ev-degree Zagreb index [12]:

$$^{*}M^{ev}(H)=\sum_{e=1}^{|E|}\frac{1}{d_X^{ev}(e)^2}. \tag{8}$$

Zagreb indices were first used to model anti-inflammatory agility in different acids [14], and then, M_1 and M_2 were used to model the clearance of cephalosporins and fraction bound in humans [15].

(i) *ve*-degree sum-connectivity index:

$$ve-SC(X)=\sum_{e=1}^{|E|}\frac{1}{\sqrt{d_X^{ve}(u)+d_X^{ve}(v)}}. \tag{9}$$

(ii) ve-degree atom-bond connectivity index:

$$ve-\mathrm{ABC}(X)=\sum_{e=1}^{|E|}\sqrt{\frac{d_X^{ve}(u)+d_X^{ve}(v)-2}{d_X^{ve}(u)\times d_X^{ve}(v)}}. \tag{10}$$

Atom-bond connectivity index is used to model heat of formation ΔH_f in alkanes [16].

(iii) ve-degree geometric arithmetic index:

$$ve-GA(X)=\sum_{e=1}^{|E|}\frac{2\sqrt{d_X^{ve}(u)\times d_X^{ve}(v)}}{d_X^{ve}(u)+d_X^{ve}(v)}. \tag{11}$$

(iv) Arithmetic-geometric index [17]:

$$ve-AG(X)=\sum_{e=1}^{|E|}\frac{d_X^{ve}(u)+d_X^{ve}(v)}{2\sqrt{d_X^{ve}(u)\times d_X^{ve}(v)}}. \tag{12}$$

In [18], the geometrical-arithmetic index (GA) was introduced and used to model the following properties of chemical compounds:

(i) Acentric factor (AcenFac)

(ii) Boiling point (BP)

(iii) Entropy (S)

(iv) Enthalpy of formation (HFORM)

(v) Enthalpy of vaporization (HVAP)

(vi) Standard enthalpy of vaporization (DHVAP)

Recently, some other topological indices (listed below) are introduced on the basis of ev- and ve-degree to model chemical properties written above which give better correlation coefficients of about 0.99088 [19].

(i) *ve*-degree harmonic index:

$$H^{ve}(X) = \sum_{e=1}^{|E|} \frac{2}{d_X^{ve}(u) + d_X^{ve}(v)}. \tag{13}$$

(ii) *ev*-degree inverse index [12]:

$$ID^{ev}(H) = \sum_{e=1}^{|E|} \frac{1}{d_X^{ev}(e)}. \tag{14}$$

(iii) ve-degree inverse sum index [20]:

$$ISI^{ve}(H) = \sum_{e=1}^{|E|} \frac{d_X^{ve}(u) \times d_X^{ve}(v)}{d_X^{ve}(u) + d_X^{ve}(v)}. \tag{15}$$

(iv) F-ev-degree index [12]:

$$F^{ev}(H) = \sum_{e=1}^{|E|} \mathrm{d}_X^{ev}(e)^3. \tag{16}$$

(v) F-ve-degree index [21]:

$$F^{ve}(H) = \sum_{e=1}^{|E|} \left(d_X^{ve}(u)^2 + d_X^{ve}(v)^2\right). \tag{17}$$

(vi) First hyper-ve-degree index [21]:

$$HM_1^{ve}(H) = \sum_{e=1}^{|E|} \left(d_X^{ve}(u) + d_X^{ve}(v)\right)^2. \tag{18}$$

(vii) Second hyper-ve-degree index [21]:

$$HM_2^{ve}(H) = \sum_{e=1}^{|E|} \left(d_X^{ve}(u) \times d_X^{ve}(v)\right)^2. \tag{19}$$

For more details, see[22–24].

2. Polyphenylene Network

Hydrocarbons, which are organic compounds formulated completely by the atoms of hydrogen and carbon elements, are one of the world's most prominent sources of energy and are found mostly in petroleum form, natural gas, and crude oil. The majority of hydrocarbons are linear chains, rings, or a mix of the two. Polyphenylene, a two-dimensional (2D) limitless hydrocarbon with the formula C_6H_4, that may be formed experimentally, is thermodynamically stable. Furthermore, due to its new structural features, 2D polyphenylene could be used in a variety of industries, such as a barrier for H_2 purification. When H_2 is produced by the conventional process of steam methane reformation, certain less desirable species are produced, such as CO, CO_2, and CH_4. As a result, isolating H_2 from these species is critical for its storage and use [25]. SRP is a superb option for many demanding applications including semiconductor components, high-performance bearings, bushings, valves, valve seats, and aircraft substructures, due to its remarkable mechanical, chemical, thermal, and electrical qualities. SRP is an ideal contender for light-weight high-performance applications due to its high specific strength. Antistatic coatings made of electrically conductive polyphenylene (p- or n-doped) are used to protect integrated circuits from static charges, humidity, and corrosion [26]. The following are important performance characteristics:

Mechanical stiffness and strength are extremely high. High compression strength and resistance to pressure, excellent wear and scratch resistance, and good cold temperature stability (to around −270°C), 155° C is a high glass transition temperature. Before and after processing, there is exceptional dimensional stability, low coefficient of thermal expansion (low thermal shrinkage), excellent acid, and basic resistance. With resistance to solvents and hot steam (but lower than PEEK), processability is good (can be extruded and injection molded).

2.1. Mathematical Work and Discussion. In this section, we will compute and discuss all the topological indices mentioned before, for the graph of polyphenylene network PN, as shown in Figure 1, where, in Figure 2, we show the unit segment of the graph. In the graph, we have vertices joined with single edge, double edges, and triple edges (i.e., $\mathrm{d}_{\mathrm{PN}}(v) \in \{1, 2, 3\}$). In the graph of polyphenylene network $\mathrm{PN}(V, E)$, we observe that there are $30m^2 + 8m - 4$ vertices and $34m^2 + m + 3$ edges. More information about the graph is given in Table 1.

Theorem 1. *Let $PN(V, E)$ be the graph of polyphenylene network; then,*

$$\begin{aligned}(a)\mathrm{ve-SC}(\mathrm{PN}) &= \left(3\sqrt{3} + \frac{5}{2\sqrt{2}} + \frac{7}{\sqrt{10}} + \frac{4}{\sqrt{15}}\right)m^2 + \frac{m}{2\sqrt{3}} - \frac{1}{2\sqrt{2}} + \frac{1}{2\sqrt{3}} + \frac{1}{\sqrt{10}} + \frac{2}{\sqrt{15}},\\ (b)\mathrm{ve-ABC}(\mathrm{PN}) &= \left(\frac{14\sqrt{2}}{5} + \sqrt{10} + 18\sqrt{2/7} + \sqrt{26/7}\right)m^2 + \sqrt{2/7}m + \frac{2\sqrt{2}}{5} - \sqrt{2/5} + \sqrt{2/7} + \sqrt{13/14}.\end{aligned} \tag{20}$$

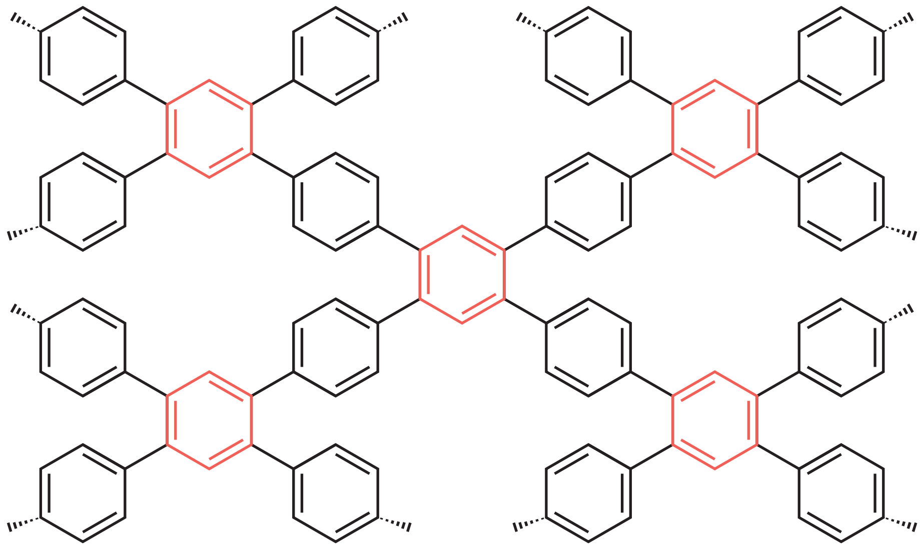

Figure 1: Molecular graph of polyphenylene network.

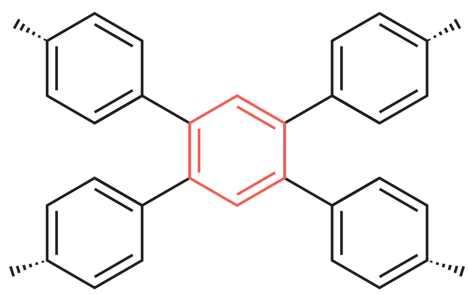

Figure 2: Unit of the graph of polyphenylene network.

Table 1: Edge partition table of polyphenylene network.

$(d_{PN}(u), d_{PN}(v))$	$d_{PN}(e)$	$(d^{ve}_{PN}(u), d^{ve}_{PN}(v))$	$d^{ev}_{PN}(e)$	Frequency
(1, 3)	2	(3, 5)	4	$5m^2-1$
(2, 2)	2	(5, 5)	4	$7m^2+1$
(2, 3)	3	(5, 7)	5	$18m^2+m+1$
(3, 3)	4	(7, 8)	6	$4m^2+2$

$$
\begin{aligned}
&(a)\ R(PN) = \frac{1}{6}(10\sqrt{3}+18\sqrt{6}+29)m^2 + \frac{m}{\sqrt{6}} + \frac{1}{6}(-2\sqrt{3}+\sqrt{6}+7),\\
&(b)\ R^{ev}(PN) = \left(2\sqrt{2/3}+\frac{18}{\sqrt{5}}+6\right)m^2 + \frac{m}{\sqrt{5}} + \sqrt{2/3} + \frac{1}{\sqrt{5}},\\
&(c)\ R^{ve}(PN) = \left(\sqrt{5/3}+\sqrt{2/7}+\frac{7}{5}+\frac{18}{\sqrt{35}}\right)m^2 + \frac{m}{\sqrt{35}} + \frac{1}{5} + \frac{1}{\sqrt{14}} - \frac{1}{\sqrt{15}} + \frac{1}{\sqrt{35}},\\
&(d)\ RR^{ev}(PN) = 2(9\sqrt{5}+2\sqrt{6}+12)m^2 + \sqrt{5}m + \sqrt{5} + 2\sqrt{6}.
\end{aligned}
\tag{21}
$$

Proof. To prove (a), we expand equation (1) and substitute values from Table 1, which gives

$$R(PN) = \frac{4m^2+2}{\sqrt{3\times 3}} + \frac{5m^2-1}{\sqrt{1\times 3}} + \frac{18m^2+m+1}{\sqrt{2\times 3}} + \frac{7m^2+1}{\sqrt{2\times 2}}$$
$$= \frac{1}{3}\left(4m^2+2\right) + \frac{1}{2}\left(7m^2+1\right) + \frac{5m^2-1}{\sqrt{3}} + \frac{18m^2+m+1}{\sqrt{6}}$$
$$= \frac{1}{6}\left((10\sqrt{3}+18\sqrt{6}+29)m^2 + \sqrt{6}m - 2\sqrt{3} + \sqrt{6} + 7\right)$$
$$= \frac{1}{6}(10\sqrt{3}+18\sqrt{6}+29)m^2 + \frac{m}{\sqrt{6}} + \frac{1}{6}(-2\sqrt{3}+\sqrt{6}+7). \tag{22}$$

To prove (b), we expand (2) and substitute values from Table 1, which gives

$$R^{ev}(PN) = \frac{4m^2+2}{\sqrt{6}} + \frac{5m^2-1}{\sqrt{4}} + \frac{18m^2+m+1}{\sqrt{5}} + \frac{7m^2+1}{\sqrt{4}}$$
$$= \frac{4m^2+2}{\sqrt{6}} + \frac{1}{2}\left(5m^2-1\right) + \frac{1}{2}\left(7m^2+1\right) + \frac{18m^2+m+1}{\sqrt{5}}$$
$$= \left(2\sqrt{2/3} + \frac{18}{\sqrt{5}} + 6\right)m^2 + \frac{m}{\sqrt{5}} + \sqrt{2/3} + \frac{1}{\sqrt{5}}. \tag{23}$$

To prove (c), we expand (3) and substitute values from Table 1, which gives

$$R^{ve}(PN) = \frac{4m^2+2}{\sqrt{7\times 8}} + \frac{5m^2-1}{\sqrt{3\times 5}} + \frac{18m^2+m+1}{\sqrt{5\times 7}} + \frac{7m^2+1}{\sqrt{5\times 5}}$$
$$= \frac{2m^2+1}{\sqrt{14}} + \frac{1}{5}\left(7m^2+1\right) + \frac{5m^2-1}{\sqrt{15}} + \frac{18m^2+m+1}{\sqrt{35}}$$
$$= \left(\sqrt{5/3}\,\sqrt{2/7} + \frac{7}{5} + \frac{18}{\sqrt{35}}\right)m^2 + \frac{m}{\sqrt{35}} + \frac{1}{5} + \frac{1}{\sqrt{14}} - \frac{1}{\sqrt{15}} + \frac{1}{\sqrt{35}}. \tag{24}$$

To prove (d), we expand (4) and substitute values from Table 1, which gives

$$RR^{ev}(PN) = \sqrt{6}\left(4m^2+2\right) + \sqrt{4}\left(5m^2-1\right) + \sqrt{5}\left(18m^2+m+1\right) + \sqrt{4}\left(7m^2+1\right)$$
$$= 2\left(5m^2-1\right) + 2\left(7m^2+1\right) + \sqrt{5}\left(18m^2+m+1\right) + \sqrt{6}\left(4m^2+2\right)$$
$$= 2(9\sqrt{5}+2\sqrt{6}+12)m^2 + \sqrt{5}m + \sqrt{5} + 2\sqrt{6}. \tag{25}$$

□

Theorem 2. *Let $PN(V,E)$ be the graph of polyphenylene network; then,*

$$\begin{aligned} &(a)\ M_i^{\text{bve}}(PN) = 386m^2 + 12m + 44,\\ &(b)\ M_{ii}^{ve}(PN) = 1104m^2 + 35m + 157,\\ &(c)\ RZG_{iii}^{ve}(PN) = 10\left(223 + 42m + 1327m^2\right),\\ &(d)\ {}^{*}M^{ev}(PN) = \frac{1}{900}\left(1423m^2 + 36m + 86\right). \end{aligned} \tag{26}$$

Proof. To prove (a), expand equation (5) and substitute values from Table 1, which gives

$$M_i^{bve}(PN) = (7+8)\left(4m^2+2\right) + (3+5)\left(5m^2-1\right) + (5+7)\left(18m^2+m+1\right)$$
$$= +(5+5)\left(7m^2+1\right)15\left(4m^2+2\right) + 8\left(5m^2-1\right) + 10\left(7m^2+1\right) + 12\left(18m^2+m+1\right)$$
$$= 386m^2 + 12m + 44. \tag{27}$$

To prove (b), expand (6) and substitute values from Table 1, which gives

$$\begin{aligned}M_{ii}^{ve}(PN) &= (7\times 8)\left(4m^2+2\right) + (3\times 5)\left(5m^2-1\right) + (5\times 7)\left(18m^2+m+1\right) + (5\times 5)\left(7m^2+1\right)\\ &= 56\left(4m^2+2\right) + 15\left(5m^2-1\right) + 25\left(7m^2+1\right) + 35\left(18m^2+m+1\right)\\ &= 1104m^2+35m+157.\end{aligned} \tag{28}$$

To prove (c), expand (7) and substitute values from Table 1, which gives

$$\begin{aligned}\mathrm{RZG}_{iii}^{ve}(PN) &= \left(5m^2-1\right)(3\times 5)(3+5) + \left(7m^2+1\right)(5\times 5)(5+5) + \left(18m^2+m+1\right)(5\times 7)(5+7) + \left(4m^2+2\right)(7\times 8)(7+8)\\ &= 840\left(2+4m^2\right) + 120\left(-1+5m^2\right) + 250\left(1+7m^2\right) + 420\left(1+m+18m^2\right)\\ &= 10\left(223+42m+1327m^2\right).\end{aligned} \tag{29}$$

To prove (d), expand (8) and substitute values from Table 1, which gives

$$\begin{aligned}* M^{ev}(PN) &= \left(5m^2-1\right)\times\frac{1}{4^2} + \left(7m^2+1\right)\times\frac{1}{4^2} + \left(18m^2+m+1\right)\times\frac{1}{5^2} + \left(4m^2+2\right)\times\frac{1}{6^2}\\ &= \frac{1}{36}\left(4m^2+2\right) + \frac{1}{16}\left(5m^2-1\right) + \frac{1}{16}\left(7m^2+1\right) + \frac{1}{25}\left(18m^2+m+1\right)\\ &= \frac{1}{900}\left(1423m^2+36m+86\right).\end{aligned} \tag{30}$$

□

Theorem 3. *Let $PN(V,E)$ be the graph of polyphenylene network; then,*

Proof. To prove (a), expanding equation (9) and substituting values from Table 1, we find

$$\begin{aligned}ve-SC(PN) &= \frac{4m^2+2}{\sqrt{7+8}} + \frac{5m^2-1}{\sqrt{3+5}} + \frac{18m^2+m+1}{\sqrt{5+7}} + \frac{7m^2+1}{\sqrt{5+5}}\\ &= \frac{4m^2+2}{\sqrt{15}} + \frac{5m^2-1}{2\sqrt{2}} + \frac{18m^2+m+1}{2\sqrt{3}} + \frac{7m^2+1}{\sqrt{10}}\\ &= \left(3\sqrt{3} + \frac{5}{2\sqrt{2}} + \frac{7}{\sqrt{10}} + \frac{4}{\sqrt{15}}\right)m^2 + \frac{m}{2\sqrt{3}} - \frac{1}{2\sqrt{2}} + \frac{1}{2\sqrt{3}} + \frac{1}{\sqrt{10}} + \frac{2}{\sqrt{15}}.\end{aligned} \tag{31}$$

To prove (b), expanding (10) and substituting values from Table 1, we find

$$\begin{aligned} ve-ABC(PN) &= \sqrt{7+8-2/7\times 8}\left(4m^2+2\right)+\sqrt{3+5-2/3\times 5}\left(5m^2-1\right)+\sqrt{5+7-2/5\times 7}\left(18m^2+m+1\right) \\ &\quad +\sqrt{5+5-2/5\times 5}\left(7m^2+1\right) \\ &= \frac{2}{5}\sqrt{2}\left(7m^2+1\right)+\sqrt{2/5}\left(5m^2-1\right)+\sqrt{2/7}\left(18m^2+m+1\right)+\sqrt{13/14}\left(2m^2+1\right) \\ &= \left(\frac{14\sqrt{2}}{5}+\sqrt{10}+18\sqrt{2/7}+\sqrt{26/7}\right)m^2+\sqrt{2/7}m+\frac{2\sqrt{2}}{5}-\sqrt{2/5}+\sqrt{2/7}+\sqrt{13/14}\$. \end{aligned} \tag{32}$$

□

Theorem 4. *Let $PN(V,E)$ be the graph of polyphenylene network, then*

$$\begin{aligned} (a)\ ve-GA(PN) &= \left(\frac{16\sqrt{14}}{15}+\frac{5\sqrt{15}}{4}+3\sqrt{35}+7\right)m^2+\frac{\sqrt{35}m}{6}+\frac{8\sqrt{14}}{15}+\frac{\sqrt{35}}{6}-\frac{\sqrt{15}}{4}+1, \\ (b)\ ve-AG(PN) &= \left(4\sqrt{\frac{5}{3}}+\frac{15}{\sqrt{14}}+\frac{108}{\sqrt{35}}+7\right)m^2+\frac{6m}{\sqrt{35}}+\frac{15}{2\sqrt{14}}-\frac{4}{\sqrt{15}}+\frac{6}{\sqrt{35}}+1. \end{aligned} \tag{33}$$

Proof. To prove (a), expand equation (11) and substitute values from Table 1, which gives

$$\begin{aligned} ve-GA(PN) &= \left(4m^2+2\right)\frac{2\sqrt{7\times 8}}{7+8}+\left(5m^2-1\right)\frac{2\sqrt{3\times 5}}{3+5}+\left(18m^2+m+1\right)\frac{2\sqrt{5\times 7}}{5+7}+\left(7m^2+1\right)\frac{2\sqrt{5\times 5}}{5+5} \\ &= 7m^2+\frac{4}{15}\sqrt{14}\left(4m^2+2\right)+\frac{1}{4}\sqrt{15}\left(5m^2-1\right)+\frac{1}{6}\sqrt{35}\left(18m^2+m+1\right)+1 \\ &= \left(\frac{16\sqrt{14}}{15}+\frac{5\sqrt{15}}{4}+3\sqrt{35}+7\right)m^2+\frac{\sqrt{35}m}{6}+\frac{8\sqrt{14}}{15}+\frac{\sqrt{35}}{6}-\frac{\sqrt{15}}{4}+1. \end{aligned} \tag{34}$$

To prove (b), expand (12) and substitute values from Table 1, which gives

$$\begin{aligned} AG^{ve}(PN) &= \left(5m^2-1\right)\frac{3+5}{2\sqrt{3\times 5}}+\left(7m^2+1\right)\frac{5+5}{2\sqrt{5\times 5}}+\left(18m^2+m+1\right)\frac{7+5}{2\sqrt{7\times 5}}+\left(4m^2+2\right)\frac{7+8}{2\sqrt{7\times 8}} \\ &= 1+7m^2+\frac{15\left(1+2m^2\right)}{2\sqrt{14}}+\frac{4\left(-1+5m^2\right)}{\sqrt{15}}+\frac{6\left(1+m+18m^2\right)}{\sqrt{35}} \\ &= \left(4\sqrt{\frac{5}{3}}+\frac{15}{\sqrt{14}}+\frac{108}{\sqrt{35}}+7\right)m^2+\frac{6m}{\sqrt{35}}+\frac{15}{2\sqrt{14}}-\frac{4}{\sqrt{15}}+\frac{6}{\sqrt{35}}+1. \end{aligned} \tag{35}$$

□

Theorem 5. *Let $PN(V,E)$ be the graph of polyphenylene network; then,*

$$H^{ve}(PN)=\frac{1}{60}\left(371m^2+10m+23\right). \tag{36}$$

Proof. To prove, expand equation (13) and substitute values from Table 1, which gives

$$\begin{aligned}H^{ve}(PN) &= \frac{2(4m^2+2)}{7+8} + \frac{2(5m^2-1)}{3+5} + \frac{2(18m^2+m+1)}{5+7} + \frac{2(7m^2+1)}{5+5}\\ &= \frac{2}{15}(4m^2+2) + \frac{1}{4}(5m^2-1) + \frac{1}{5}(7m^2+1) + \frac{1}{6}(18m^2+m+1)\\ &= \frac{1}{60}(371m^2+10m+23).\end{aligned} \tag{37}$$

□

Theorem 6. *Let* $PN(V,E)$ *be the graph of polyphenylene network; then,*

$$\begin{aligned}&(a)\ ID^{ev}(PN) = \frac{1}{15}(109m^2+3m+8),\\ &(b)\ \mathrm{ISI}^{ve}(PN) = \frac{1}{120}(1321+350m+11317m^2).\end{aligned} \tag{38}$$

Proof. To prove (a), expand equation (14) and substitute values from Table 1, which gives

$$\begin{aligned}ID^{ev}(PN) &= (5m^2-1)\times\frac{1}{4} + (7m^2+1)\times\frac{1}{4} + (18m^2+m+1)\times\frac{1}{5} + (4m^2+2)\times\frac{1}{6}\\ &= \frac{1}{15}(109m^2+3m+8).\end{aligned} \tag{39}$$

To prove (b), expand (15) and substitute values from Table 1, which gives

$$\begin{aligned}\mathrm{ISI}^{ve}(PN) &= (5m^2-1)\frac{3\times5}{3+5} + (7m^2+1)\frac{5\times5}{5+5} + (18m^2+m+1)\frac{7\times5}{7+5} + (4m^2+2)\frac{7\times8}{7+8}\\ &= \frac{56}{15}(2+4m^2) + \frac{15}{8}(-1+5m^2) + \frac{5}{2}(1+7m^2) + \frac{35}{12}(1+m+18m^2)\\ &= \frac{1}{120}(1321+350m+11317m^2).\end{aligned} \tag{40}$$

□

Theorem 7. *Let* $PN(V,E)$ *be the graph of polyphenylene network; then,*

$$\begin{aligned}&(a)\ F^{ev}(PN) = 3882m^2+125m+557,\\ &(b)\ F^{ve}(PN) = 316+74m+2304m^2.\end{aligned} \tag{41}$$

Proof. To prove (a), expand equation (16) and substitute values from Table 1, which gives

$$\begin{aligned}F^{ev}(PN) &= 4^3(5m^2-1) + 4^3(7m^2+1) + 5^3(18m^2+m+1) + 6^3(4m^2+2)\\ &= 216(4m^2+2) + 64(5m^2-1) + 64(7m^2+1) + 125(18m^2+m+1)\\ &= 3882m^2+125m+557.\end{aligned} \tag{42}$$

Table 2: The numerical representation of Randic-type indices.

m	R(PN)	R^{ev}(PN)	R^{ve}(PN)	RR^{ev}(PN)
1	16.474 4	17.393 8	6.815 2	83.418 3
2	62.088 3	64.889 5	25.788 4	307.796
3	137.839	143.751	57.297 8	680.268
4	243.727	253.978	101.343	1200.83
5	379.753	395.571	157.925	1869.49
6	545.915	568.529	227.043	2686.25
7	742.214	772.853	308.697	3651.1
8	968.651	1008.54	402.887	4764.04
9	1225.22	1275.6	509.613	6025.08
10	1511.94	1574.02	628.876	7434.21

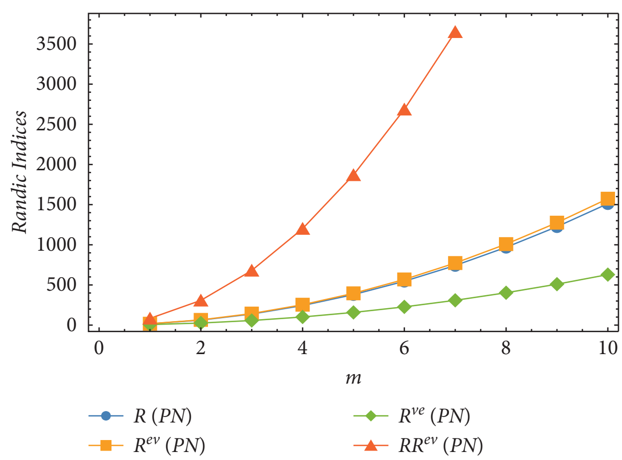

Figure 3: The graphical representation of Randic-type indices.

Table 3: The numerical representation of Zagreb-type indices.

m	M_{i}^{bve}(PN)	M_{ii}^{ve}(PN)	RZG_{iii}^{ve}(PN)	$*M^{ve}$(PN)
1	442	1296	15 920	1.716 67
2	1612	4643	56 150	6.5
3	3554	10 198	122 920	14.445 6
4	6268	17 961	216 230	25.553 3
5	9754	27 932	336 080	39.823 3
6	14 012	40 111	482 470	57.255 6
7	19 042	54 498	655 400	77.85
8	24 844	71 093	854 870	101.607
9	31 418	89 896	1080 880	128.526
10	38 764	110 907	1333 430	158.607

To prove (b), expand (17) and substitute values from Table 1, which gives

$$\begin{aligned} F^{ve}(PN) &= \left(5m^2-1\right)\left(3^2+5^2\right)+\left(7m^2+1\right)\left(5^2+5^2\right)+\left(18m^2+m+1\right)\left(5^2+7^2\right)+\left(4m^2+2\right)\left(7^2+8^2\right) \\ &= 113\left(2+4m^2\right)+34\left(-1+5m^2\right)+50\left(1+7m^2\right)+74\left(1+m+18m^2\right) \\ &= 316+74m+2304m^2. \end{aligned} \tag{43}$$

□

Theorem 8. *Let $PN(V,E)$ be the graph of polyphenylene network; then,*

$$\begin{aligned} &(a)\ HM_1^{ve}(PN)=6\left(105+24m+752m^2\right), \\ &(b)\ HM_2^{ve}(PN)=7897+1225m+40094m^2. \end{aligned} \tag{44}$$

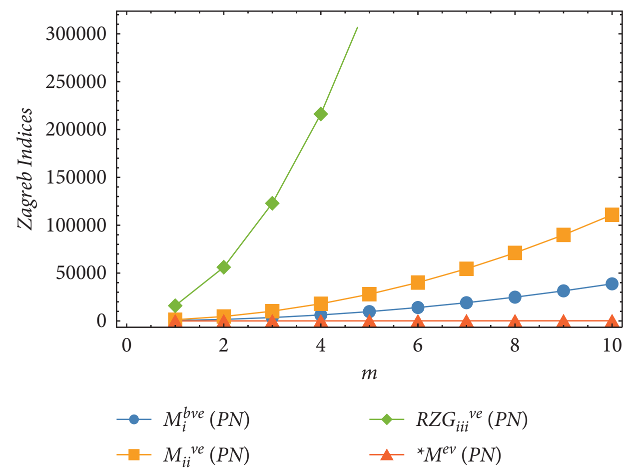

Figure 4: The graphical representation of Zagreb-type indices.

Table 4: The numerical representation of ve-ABC and ve-SC indices.

m	ve - ABC(PN)	ve - SC(PN)
1	20.6366	11.2667
2	77.1833	42.1863
3	171.072	93.5266
4	302.301	165.287
5	470.872	257.469
6	676.785	370.071
7	920.039	503.094
8	1200.63	656.537
9	1518.57	830.401
10	1873.85	1024.69

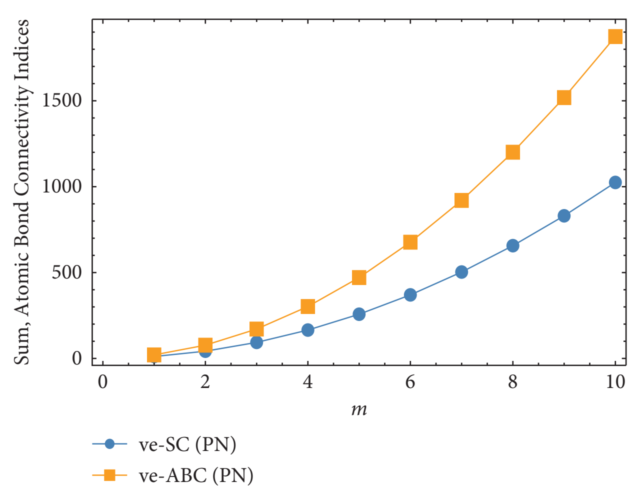

Figure 5: The graphical representation of ve-ABC and ve-SC indices.

Proof. To prove (a), expand equation (18) and substitute values from Table 1, which gives

$$\begin{aligned} HM_1^{ve}(PN) &= \left(5m^2-1\right)(3+5)^2+\left(7m^2+1\right)(5+5)^2+\left(18m^2+m+1\right)(5+7)^2+\left(4m^2+2\right)(7+8)^2 \\ &= 225\left(2+4m^2\right)+64\left(-1+5m^2\right)+100\left(1+7m^2\right)+144\left(1+m+18m^2\right) \\ &= 6\left(105+24m+752m^2\right). \end{aligned} \tag{45}$$

Table 5: The numerical representation of the geometric arithmetic index.

m	ve - GA(PN)	ve - AG(PN)
1	37.579 9	38.428 3
2	139.308	142.727
3	308.196	315.882
4	544.246	557.894
5	847.458	868.762
6	1217.83	1248.49
7	1655.36	1697.07
8	2160.06	2214.51
9	2731.91	2800.8
10	3370.93	3455.95

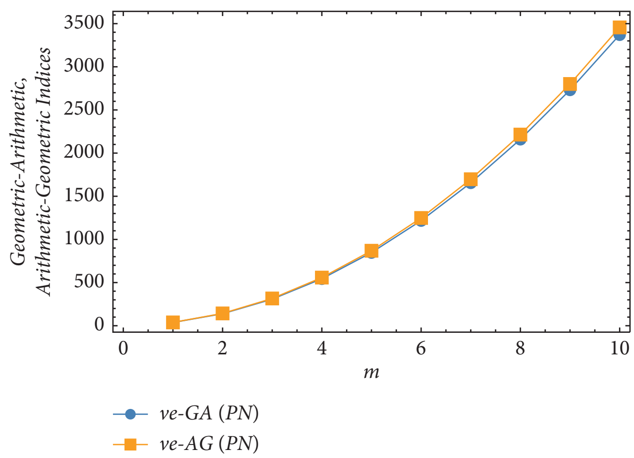

Figure 6: The graphical representation of the geometric arithmetic index.

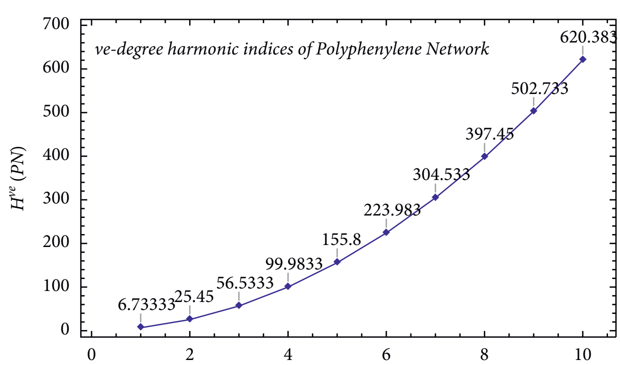

Figure 7: The graphical representation of ve-degree harmonic indices.

Table 6: The numerical representation of inverse indices.

m	ID^{ev} (PN)	ISI^{ve} (PN)
1	8	108.233
2	30	394.075
3	66.533 3	868.533
4	117.6	1531.61
5	183.2	2383.3
6	263.333	3423.61
7	358	4652.53
8	467.2	6070.07
9	590.933	7676.23
10	729.2	9471.01

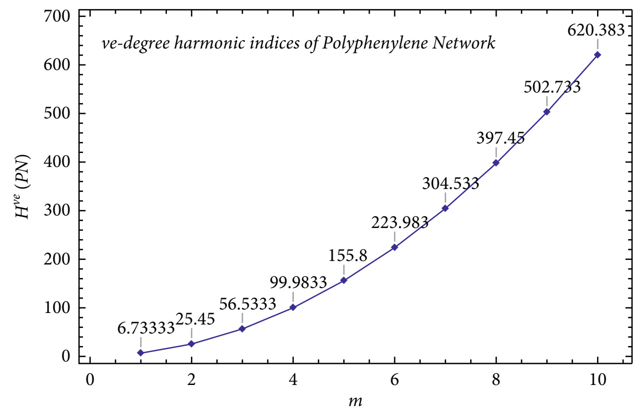

Figure 8: The graphical representation of inverse indices.

Table 7: The numerical representation of F-ev-degree index.

m	F^{ev} (PN)	F^{ve} (PN)
1	4564	2694
2	16 335	9680
3	35 870	21 274
4	63 169	37 476
5	98 232	58 286
6	141 059	83 704
7	191 650	113 730
8	250 005	148 364
9	316 124	187 606
10	390 007	231 456

To prove (b), expand (19) and substitute values from Table 1, which gives

$$\begin{aligned} HM_2^{ve}(PN) &= \left(5m^2-1\right)(3\times 5)^2+\left(7m^2+1\right)(5\times 5)^2+\left(18m^2+m+1\right)(5\times 7)^2+\left(4m^2+2\right)(7\times 8)^2 \\ &= 3136\left(2+4m^2\right)+225\left(-1+5m^2\right)+625\left(1+7m^2\right)+1225\left(1+m+18m^2\right) \\ &= 7897+1225m+40094m^2. \end{aligned} \tag{46}$$

□

2.2. Numerical and Graphical Discussion. In Theorem 1, we stated and then computed Randić indices of the graph of polyphenylene network (Figure 1) for m frameworks or units. By the resulting equations, we determined exact numerical values of Randić indices, for some $m(=1,2,\ldots,10)$, and listed in Table 2 and plotted them in Figure 3 by which we can observe that all the resulting equations show parabolic behavior. For continuously increasing values of m, all the indices go to infinity. RR^{ev} (PN) increases faster than other indices which are in order $R^{ve}(\text{PN}) < R(\text{PN}) < R^{ev}(\text{PN})$.

Table 3 and Figure 4 are derived from Theorem 2 which show the numerical values and graphical pattern of the Zagreb indices of polyphenylene network. The curves are parabolic, and the parabola for RZG_{iii}^{ve} (PN) has the shortest length of lactusrectum; i.e., it runs much faster than the others.

In Table 4 and Figure 5, we exhibited the numerical measures and graphical style of sum-connectivity and atom-bond connectivity indices from Theorem 3. The curves are parabolic, and the separation between them becomes greater and greater for increasing values of m.ve – ABC (PN) earns larger numerical value than ve – SC (PN) for all values of m.

For m units of polyphenylene, ve – GA (PN) and ve – AG (PN) were given in Theorem 4. By substituting $m=1,\ldots,10$, Table 5 is constructed. In Figure 6, the curves of both the indices are shown from where we can observe that the span between them is growing gradually.

In Figure 7, the outcomes of Theorem 5 are shown. The numerical values are increasing continuously with the increase of frameworks m.

Table 6 and Figure 8 are established for Theorem 6 in which we can see that, for all m, $ID^{ev}(\text{PN}) < ISI^{ve}(\text{PN})$, and

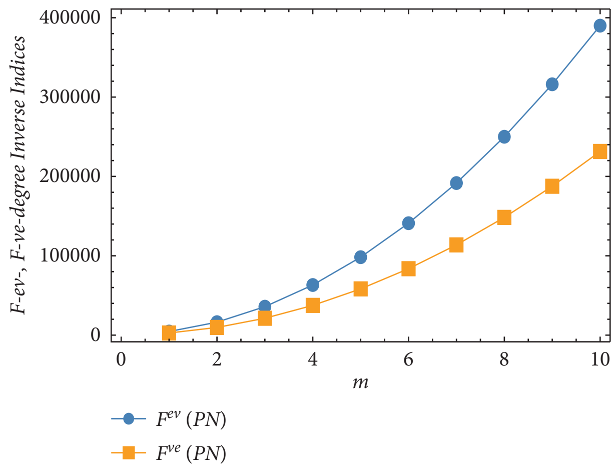

Figure 9: The graphical representation of F-ev-degree index.

Table 8: The numerical representation of hyper-ve-degree index.

m	$HM_1^{ve}(PN)$	$HM_2^{ve}(PN)$
1	5286	49 216
2	18 966	170 723
3	41 670	372 418
4	73 398	654 301
5	114 150	1.01637×10^6
6	163 926	1.45863×10^6
7	222 726	1.98108×10^6
8	290 550	2.58371×10^6
9	367 398	3.26654×10^6
10	453 270	4.02955×10^6

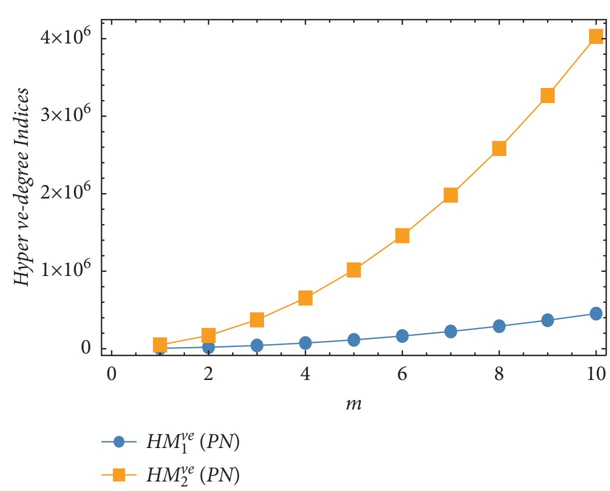

Figure 10: The graphical representation of hyper-ve-degree index.

both the curves are parabolic in manner. The span between the curves is growing very high.

Numerical values of the indices discussed in Theorem 7 are given in Table 7, where the graph of both the indices is shown in Figure 9. Again, both the curve are parabolic. The index F^{ev}(PN) acquires higher values than the index F^{ve}(PN) all the time, for the graph of polyphenylene network.

Following are the conclusions of final Theorem 8. The numerical representation is shown in Table 8, and graphical representation is shown in Figure 10. Once again both the curves are parabolic. The separation between them is growing continuously. The numerical values of $HM_1^{ve}(PN)$ is always less than the numerical values of $HM_2^{ve}(PN)$.

3. Conclusion

In this study, we calculated 19 topological indices discussed in Section 1 for the graph of polyphenylene network. Each index represents a unique chemical or physical property which is also mentioned in section 1. We also mentioned many qualities of polyphenylene which tell that it is an admirable chemical compound to make new substances and to improve dispositions of the present one. Therefore, the work of this paper will provide assistance in studying the properties of polyphenylene and its derivatives.

Data Availability

The data used to support the findings of this study are cited at relevant places within the article as references.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

All authors equally contributed to this work.

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