ZEROTH-ORDER GENERAL RANDIĆ INDEX OF LINE GRAPHS OF SOME CHEMICAL STRUCTURES IN DRUGS

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Zeroth-order general Randić index of drug molecular structures is beneficial for medical and pharmaceutical researchers because it is significant of testing the chemical and pharmacological characteristics of drug molecular structures that can make up the defects of chemical and medicine experiments and can provide the theoretical basis for the manufacturing of drugs in pharmaceutical engineering. In this paper, we establish general expressions for evaluating the zeroth-order general Randić index of line graphs of various well-known chemical structures. The established results may be useful to determine physicochemical properties and biological activities of the considered chemical structures in drugs.

Keywords: Computational medical, Zeroth-order general Randić index, Line graphs, Dendrimer stars, Bridge graph, Benzenoid series

List of Notations:

Notation	Description
$V(G)$	Vertex set of a molecular graph G
$E(G)$	Edge set of a molecular graph G
R	Randić index
${}^0R$	Zeroth-order Randić index
${}^0R_\alpha$	Zeroth-order general Randić index
$\delta(G)$	Minimum degree of a molecular graph G
$\Delta(G)$	Maximum degree of a molecular graph G
$L(G)$	Line graph of a molecular graph G
$d(v)$	Degree of a vertex

1. Introduction

As we move into the new millennium it is becoming increasingly clear that the biomedical sciences are entering the most exciting phase of their development. Technological developments in medicine manufacturing, chemical and

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pharmaceutical techniques have been promptly evolved and a large number of new nano-materials, crystalline materials and drugs emerge every year. Enormous amount of chemical experiments and work is mandatory to determine the chemical properties of new compounds and drugs to test their physical features, chemical reactivity, and biological activity. Advanced equipment, sufficient reagents and human resources are required to investigate the performance and the reaction of these new drugs but in lower income areas and in poor countries where enough money is lacked to afford the relevant chemical reagents and equipment to measure their biochemical and pharmaceutical properties, have to face severe problem.

The main paradigm of medicinal chemistry is that biological activity, as well as physical and chemical properties of organic compounds such as melting point, boiling point, and toxicity of drugs, is inherent on their molecular structures. Chemical graph theory (CGT) or molecular topology is the branch of mathematical chemistry which deals with the study of molecular structures and nontrivial implementation of graph theory to solve problems regarding to the chemical structures. Topological descriptor has strong correspondence with a molecular property; it can be named as molecular index or topological index (TI). There are various well-known topological indices applied in chemical engineering (e.g., QSPR/QSAR study) for grasping the relationships between the molecular structure and the potential physicochemical characteristics. If we enumerate indicators of the drug molecular structures in accordance with the topological indices, the medical and pharmaceutical researchers could find it beneficial to well know the medicinal and chemical properties of new manufactured drugs. From this perspective, we can appreciate the effectiveness of the methods of computing topological indices especially for developing countries which lack inadequate money and funds and where the available biological and medical information about new drugs may be easily obtained without the need to carry out chemical experiments and purchase expensive equipment and reagents.

For convenience of our discussion about medicine mathematical model, we first recall some relevant terminologies and notations, which can be found in [4] with clear explanation. Conventionally the structure of a drug is considered as an undirected (chemical) graph where each vertex expresses an atom and each edge represents a chemical bond between these atoms. We consider G as a simple graph corresponding to a drug structure with an atom (vertex) set as $V(G)$ and a chemical bond (edge) set as $E(G)$. Topological index of a molecule structure can be considered as a non-empirical numerical quantity which quantitates the molecular structure and its branching pattern. In this point of view, it is used as a descriptor of the molecule under testing. A topological index defined on the molecule structure G can be regarded as a real-valued function f:

$G \rightarrow R^+$ which maps each drug molecular structure to certain real numbers. Researchers have built up noteworthy indices decades prior that have wide-ranging applications in the correlation and prediction of various molecular properties and furthermore in trial of similarity and isomorphism of the drug molecules [5]. Several reports help to determine the topological indices of special molecular graphs in chemical, nanomaterials and pharmaceutical engineering which help researchers to understand the physical features, chemical reactivity and biological activity of their corresponding molecular structures.

The chemist Milan Randić [23] established a topological index named as Randić index that is worthy for determining the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. The Randić index is defined as:

$$\mathrm{R} = \mathrm{R}(G) = \sum_{uv \in E(G)} [d(u)d(v)]^{-\frac{1}{2}},$$

where $d(u)$ denotes the degree of the vertex u of the graph G, $E(G)$ is the edge set of G and the summation goes over all edges of G. Randić himself demonstrated that his index is strongly correlated with several physico-chemical properties of alkanes: boiling points, chromatographic retention times, enthalpies of formation, parameters in the Antoine equation for vapor pressure, surface areas, etc. [20]. Eventually R become one of the most famous molecular descriptors to which two books [14] and [16], several reviews and countless research papers are devoted. Bollobás and Erdös [3] generalized R(G) by replacing the exponent $\frac{-1}{2}$ by an arbitrary real number α . This graph invariant is called the general Randić index and will be denoted by:

$$\mathrm{R}_\alpha = \mathrm{R}_\alpha(G) = \sum_{uv \in E(G)} [d(u)d(v)]^{\alpha},$$

The zeroth-order Randić index ${}^0\mathrm{R}$ defined by Kier and Hall [15], is:

$${}^0\mathrm{R}(G) = \sum_{v \in V(G)} [d(v)]^{-\frac{1}{2}},$$

where the summation goes over all vertices of G. Kier and Hall gave a general scheme based on the Randić index to also calculate zeroth-order ${}^0\mathrm{R}$ and higher-order connectivity indices ${}^m\mathrm{R}$.

Eventually, Li and Zheng [19] introduced a new index of a graph G and named it zeroth-order general Randić index, which is based on vertex degrees of graphs. Like other successful structure-descriptors, this index received considerable recognition from mathematical chemists and mathematicians, and it is very popular topological index in mathematical chemistry. Let $G = (V, E)$ be a

graph with the vertex set $V(G)$ and the edge set $E(G)$. The zeroth-order general Randić index ${}^0\mathrm{R}(G)$ is defined as:

$$ {}^0\mathrm{R}_\alpha(G) = \sum_{v \in V(G)} [d(v)]^\alpha, $$

where α is an arbitrary real number and $d(v)$ is denoted as the degree of vertex v (the number of vertex adjacent to vertex v) [13]. It was discovered that zeroth-order general Randić index has some outstanding applications or unexpected mathematical properties. Pavlović [22] determined the graphs with maximum ${}^0\mathrm{R}$-index. Lang et al. [18] investigated the same problem for the topological index M_1 where $M_1 \equiv {}^0\mathrm{R}_\alpha$ for α = +2. This success encouraged researchers to search for mathematical properties of the zeroth-order general Randić index.

Let the vertex set $V(G)$ can be divided into several partitions such that V_i represents a vertex having degree i and $v_i = |V_i|$. Line graph $L(G)$ of a graph G has the vertex set $V(L(G)) = E(G)$ where the two distinct vertices of $L(G)$ are adjacent if the corresponding edges of G are adjacent.

With continued work on Gao et al. [10] we obtained the zeroth-order general Randić index of line graphs of various essential chemical structures in drugs.

2. Zeroth-order general Randić index of line graph of graphene G(m, n)

Graphene is a one-atom thick and single tightly packed sheet of hexagonally arranged carbon atoms. It is a two-dimensional layer of honeycomb lattice, in which carbon atoms are bonded together in a repeating pattern of hexagons, with each carbon atom covalently bonded to three other carbon atoms. It is the thinnest material possible as well as being transparent. It is the main element of certain carbon allotropes including charcoal, fullerenes and graphite etc. Graphene is undoubtedly emerging as one of the most promising nanomaterials as it is extraordinarily strong, supernaturally light, and electrically super-conductive. See Shigehalli and Kanabur [24] for more details.

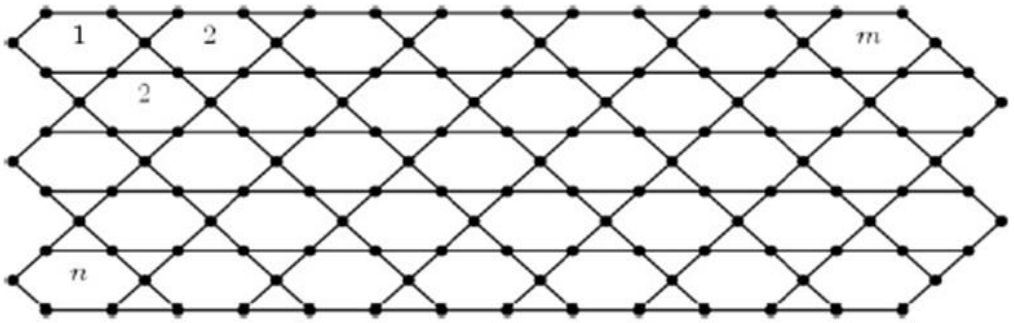

Fig. 1. 2-Dimensional line graph of graphene sheet.

Theorem 1. The zeroth-order general Randić index of line graph of $G(m, n)$ is:

$$ {}^{0}\mathrm{R}_{\alpha}\left(L(G(m,n))\right) = \begin{cases} [4(3^{\alpha})+4^{\alpha}]m+[6(2^{\alpha})-4(3^{\alpha})-4^{\alpha}]; & for\, n=1 \\ 3(4^{\alpha})mn+2[2(3^{\alpha})-4^{\alpha}]m+[2^{\alpha}+2(3^{\alpha})-4^{\alpha}]n & \\ +[4(2^{\alpha})-4(3^{\alpha})-4^{\alpha}]; & for\, n\geq 2 \end{cases} $$

where $G(m, n)$ is a molecular graph of graphene with n rows and m columns. α is any real number.

Proof. By analyzing the molecular structure of the line graph of graphene $G(m,n)$*:* For $n = 1$: we infer $v_2 = 6$, $v_3 = 4m - 4$ and $v_4 = m - 1$. Therefore, using the definition of zeroth-order general Randić index, we obtain

$$\begin{aligned} {}^{0}\mathrm{R}_{\alpha}(L(G(m,n))) &= \sum_{v\in V(L(G(m,n)))}[d(v)]^{\alpha} \\ &= \sum_{v\in V_2}(2)^{\alpha}+\sum_{v\in V_3}(3)^{\alpha}+\sum_{v\in V_4}(4)^{\alpha} \\ &= 2^{\alpha}(6)+3^{\alpha}(4m-4)+4^{\alpha}(m-1) \\ &= [4(3^{\alpha})+4^{\alpha}]m+[6(2^{\alpha})-4(3^{\alpha})-4^{\alpha}]. \end{aligned}$$

For $n \geq 2$: we infer $v_2 = n + 4$, $v_3 = 4m + 2n - 4$ and $v_4 = 3mn - 2m - n - 1$. Similarly, by using the definition of zeroth-order general Randić index, we obtain

$$\begin{aligned} {}^{0}\mathrm{R}_{\alpha}(L(G(m,n))) &= \sum_{v\in V(L(G(m,n)))}[d(v)]^{\alpha} \\ &= \sum_{v\in V_2}(2)^{\alpha}+\sum_{v\in V_3}(3)^{\alpha}+\sum_{v\in V_4}(4)^{\alpha} \\ &= 2^{\alpha}(n+4)+3^{\alpha}(4m+2n-4)+4^{\alpha}(3mn-2m-n-1) \\ &= 3(4^{\alpha})mn+2[2(3^{\alpha})-4^{\alpha}]m+[2^{\alpha}+2(3^{\alpha})-4^{\alpha}]n+[4(2^{\alpha})-4(3^{\alpha})-4^{\alpha}]. \end{aligned}$$

□

3. Zeroth-order general Randić index of line graph of three family of dendrimer stars

Dendrimers are large and complex molecules with very well-defined chemical structures. They are produced in an iterative sequence of reaction steps. The nanostar dendrimers are part of a new group of macromolecules with a precise tailored architecture. These are hyper-branched nanostructures that can be synthesized by divergent or convergent methods, and they are developed from branched units referred to as monomers using a nanoscale fabrication method. In this section, we determine the zeroth-order general Randić index of line graphs of three famous infinite classes $NS_1[n]$, $NS_2[n]$ and $NS_3[n]$ of dendrimer stars which widely appear in the drug structures. For detailed structure, see Ashrafi and Nikzad [1].

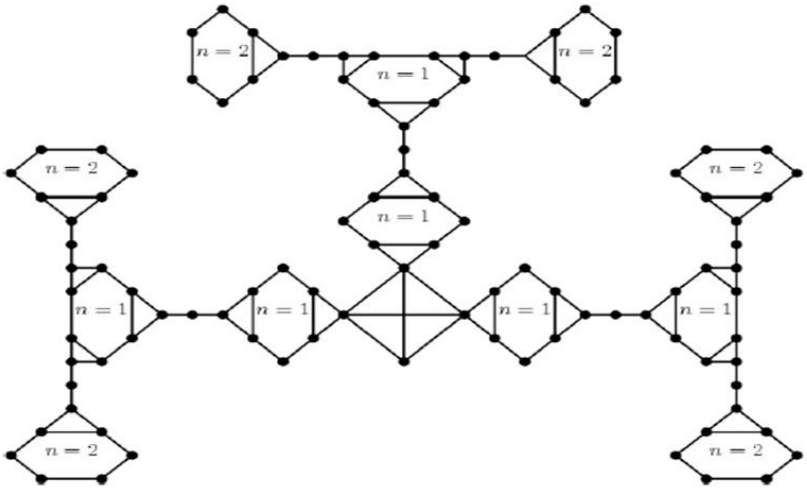

Fig. 2.1. Line graph of the first type of nanostar dendrimer $L(NS_1[2])$.

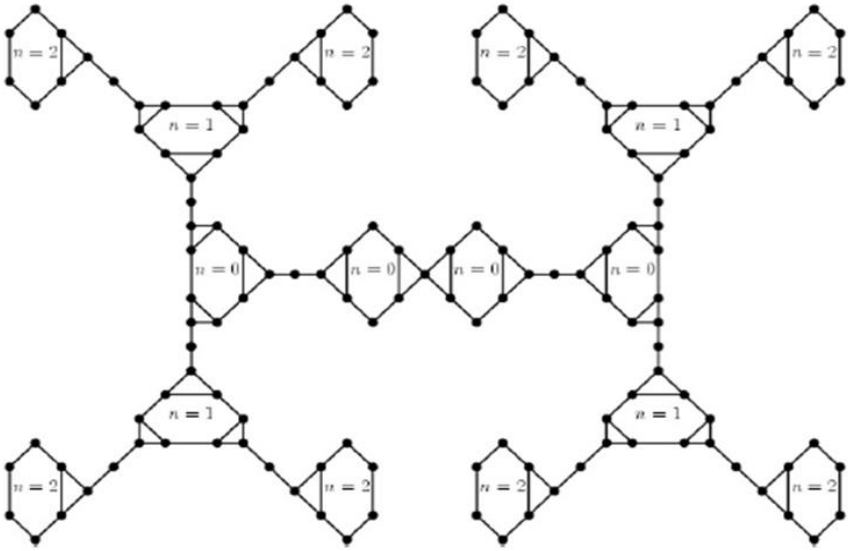

Fig. 2.2. Line graph of the second type of nanostar dendrimer $L(NS_2[2])$.

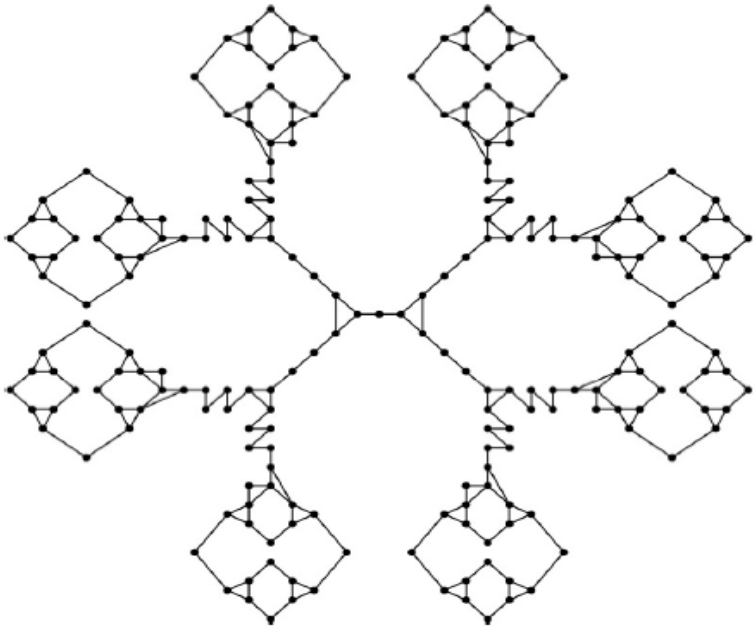

Fig. 2.3. Line graph of the third type of nanostar dendrimer $L(NS_3[2])$.

Theorem 2. The zeroth-order general Randić index of line graphs of three infinite classes $NS_1[n]$, $NS_2[n]$ and $NS_3[n]$ of dendrimer stars is:

$$^0\mathrm{R}_\alpha(L(NS_1[n])) = 9[2^\alpha + 2(3^\alpha)]2^n + [3(2^\alpha) - 11(3^\alpha) + 3(5^\alpha)].$$

$$^0\mathrm{R}_\alpha(L(NS_2[n])) = 12[2^\alpha + 2(3^\alpha)]2^n + [2(2^\alpha) - 8(3^\alpha) + 4^\alpha].$$

$$^0\mathrm{R}_\alpha(L(NS_3[n])) = 2[12(2^\alpha) + 14(3^\alpha) + 3(4^\alpha)]2^n - [7(2^\alpha) + 6(3^\alpha)].$$

where *n* is the number of steps of growth of these three family of dendrimer stars and α is any real number.

Proof. By observing the structures of the line graphs of these three infinite classes of dendrimer stars, we deduce its vertex partition with respect to the degrees as follows:

- For $L(NS_1[n])$: $v_2 = 9(2^n) + 3$, $v_3 = 18(2^n) - 11$ and $v_5 = 3$.
- For $L(NS_2[n])$: $v_2 = 12(2^n - 1) + 14$, $v_3 = 24(2^n - 1) + 16$ and $v_4 = 1$.
- For $L(NS_3[n])$: $v_2 = 48(2^{n-1} - 1) + 41$, $v_3 = 56(2^{n-1} - 1) + 50$ and $v_4 = 12(2^{n-1})$.

Therefore, according to the definition of zeroth-order general Randić index, we check

$$\begin{aligned}
^0\mathrm{R}_\alpha(L(NS_1[n])) &= \sum_{v\in V(L(NS_1[n]))} [d(v)]^\alpha \\
&= \sum_{v\in V_2} (2)^\alpha + \sum_{v\in V_3} (3)^\alpha + \sum_{v\in V_5} (5)^\alpha \\
&= 2^\alpha[9(2^n) + 3] + 3^\alpha[18(2^n) - 11] + 5^\alpha(3) \\
&= 9[2^\alpha + 2(3^\alpha)]2^n + [3(2^\alpha) - 11(3^\alpha) + 3(5^\alpha)].
\end{aligned}$$

$$\begin{aligned}
^0\mathrm{R}_\alpha(L(NS_2[n])) &= \sum_{v\in V(L(NS_2[n]))} [d(v)]^\alpha \\
&= \sum_{v\in V_2} (2)^\alpha + \sum_{v\in V_3} (3)^\alpha + \sum_{v\in V_4} (4)^\alpha \\
&= 2^\alpha[12(2^n - 1) + 14] + 3^\alpha[24(2^n - 1) + 16] + 4^\alpha(1) \\
&= 12[2^\alpha + 2(3^\alpha)]2^n + [2(2^\alpha) - 8(3^\alpha) + 4^\alpha].
\end{aligned}$$

$$
\begin{aligned}
{}^{0}\mathrm{R}_{\alpha}(L(NS_3[n])) &= \sum_{v\in V(L(NS_3[n]))} [d(v)]^{\alpha} \\
&= \sum_{v\in V_2} (2)^{\alpha} + \sum_{v\in V_3} (3)^{\alpha} + \sum_{v\in V_4} (4)^{\alpha} \\
&= 2^{\alpha}[48(2^{n-1}-1)+41] + 3^{\alpha}[56(2^{n-1}-1)+50] + 4^{\alpha}[12(2^{n-1})] \\
&= 2[12(2^{\alpha}) + 14(3^{\alpha}) + 3(4^{\alpha})]2^{n} - [7(2^{\alpha}) + 6(3^{\alpha})].
\end{aligned}
$$

□

4. Zeroth-order general Randić index of line graph of polyomino chains of *n*-cycles

"A *k*-polyomino system is a finite 2-connected plane graph such that each interior face (also called cell) is surrounded by a regular 4*k*-cycle (C_{4k}) of length one. In other words, it is an edge-connected union of cells in the planar square lattice" [12]. This polyomino system divides the plane into one infinite external region and a number of finite internal regions where all internal regions must be squares. For the origin of polyominoes and more details can be found in Klarner and Polyominoes [17], Ghorbani and Ghazi [12] and Mansour and Schork [21].

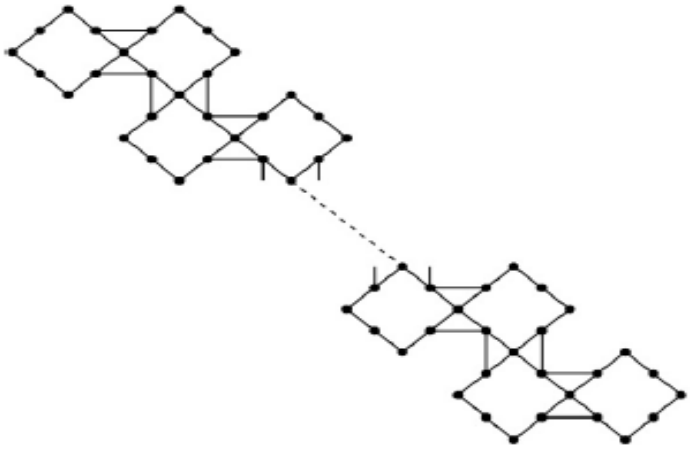

Fig. 3. Line graph of the zig-zag chain of 8-cycles.

Theorem 3. The zeroth-order general Randić index of line graph of polyomino chain of 8-cycles is:

$$
{}^{0}\mathrm{R}_{\alpha}(L(G)) = 4[3(2^{\alpha}) + 2(3^{\alpha}) + 2(4^{\alpha})]n + [4(2^{\alpha}) - 3(4^{\alpha})].
$$

where *G* is a molecular graph of the zig-zag chain of 8-cycles and α is any real number.

Proof. By means of structure analysis of line graph of the zig-zag chain of 8-cycles, we infer $v_2 = 12n + 4$, $v_3 = 8n$ and $v_4 = 8n - 3$. Therefore, using the definition of zeroth-order general Randić index, we obtain

$$\begin{aligned}
{}^0\mathrm{R}_\alpha(L(G)) &= \sum_{v\in V(L(G))} [d(v)]^\alpha \\
&= \sum_{v\in V_2} (2)^\alpha + \sum_{v\in V_3} (3)^\alpha + \sum_{v\in V_4} (4)^\alpha \\
&= 2^\alpha(12n+4) + 3^\alpha(8n) + 4^\alpha(8n-3) \\
&= 4[3(2^\alpha) + 2(3^\alpha) + 2(4^\alpha)]n + [4(2^\alpha) - 3(4^\alpha)].
\end{aligned}$$

□

5. Zeroth-order general Randić index of line graph of triangular benzenoid

The benzene molecule is a usual molecule in chemistry, physics and nano-sciences and is very useful to synthesize aromatic compounds. Triangular benzenoid denoted by $T(n)$ is a family of benzenoid molecular graphs, which is the generalization of benzene molecule C_6H_6 in which benzene rings form a triangular shape. Triangular benzenoid consists of hexagons arranged in rows and in each row one hexagon increases. Details related to its structure can be found in Ghorbani and Ghazi [12].

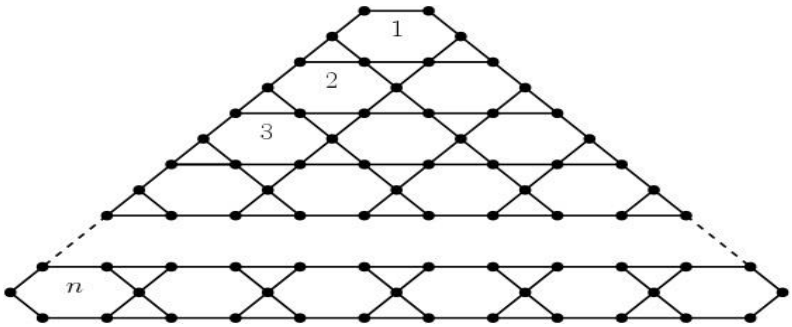

Fig. 4. Line graph of triangular benzenoid $L(T(n))$.

Theorem 4. The zeroth-order general Randić index of line graph of $T(n)$ is:

$${}^0\mathrm{R}_\alpha(L(T(n))) = [\frac{3}{2}(4^\alpha)]n^2 + 3[2(3^\alpha) - \frac{1}{2}(4^\alpha)]n + 6(2^\alpha - 3^\alpha).$$

where $T(n)$ is a molecular graph of triangular benzenoid and α is any real number.

Proof. Using the vertex dividing technique for the line graph of triangular benzenoid, we derive $v_2 = 6$, $v_3 = 6(n - 1)$ and $v_4 = \frac{3}{2}(n^2 - n)$. Hence, by definition of zeroth-order general Randić index, we get

$$
\begin{aligned}
{}^{0}\mathrm{R}_{\alpha}(L(T(n))) &= \sum_{v \in V(L(T(n)))} [d(v)]^{\alpha} \\
&= \sum_{v \in V_2} (2)^{\alpha} + \sum_{v \in V_3} (3)^{\alpha} + \sum_{v \in V_4} (4)^{\alpha} \\
&= 2^{\alpha}(6) + 3^{\alpha}[6(n-1)] + 4^{\alpha}[\frac{3}{2}(n^2 - n)] \\
&= [\frac{3}{2}(4^{\alpha})]n^2 + 3[2(3^{\alpha}) - \frac{1}{2}(4^{\alpha})]n + 6(2^{\alpha} - 3^{\alpha}).
\end{aligned}
$$

□

6. Zeroth-order general Randić index of line graph of bridge molecular structures

"Let's consider $\{G_i\}_{i=1}^{d}$ be a set of finite pairwise disjoint molecular graphs with $v_i \in V(G_i)$. The bridge molecular graph $B(G_1, \ldots, G_d) = B(G_1, \ldots, G_d; v_1, \ldots, v_d)$ of $\{G_i\}_{i=1}^{d}$ with regard to the vertices $\{v_i\}_{i=1}^{d}$ is acquired from the molecular graphs $G_1, \ldots, G_d$ in which the vertices v_i and $v_i + 1$ are attached through an edge from $i = 1, 2, \ldots, d - 1$. In this section we determine the formulas of some degree-based indices for the line graphs of infinite family of drug structures of the bridge molecular graph with $G_1, \ldots, G_d$" [10]. Then we established $L(G_d(H, v)) = L(B(H, \ldots, H; v, \ldots, v))$ for particular cases of the bridge molecular graphs.

We analyze the line graphs of bridge molecular graphs as follows and the main parts of the graphs are path, cycle and complete molecular graph, respectively. See Gao et al. [10] and [11] for more structural details.

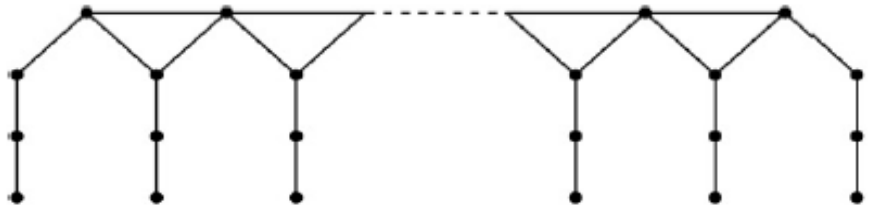

Fig. 5.1. Line graph of the bridge molecular graph $L(G_d(P_n, v))$.

Theorem 5.1. The zeroth-order general Randić index of line graph of $G_d(P_n, v)$ is:

$$ {}^{0}\mathrm{R}_{\alpha}\left(L(G_d(P_n,v))\right) = \begin{cases} 2(2^{\alpha})n - 3(2^{\alpha}) + 2; & for\, d = 2\, and\, n \geq 2 \\ (2^{\alpha} + 4^{\alpha})d + [2(3^{\alpha}) - 2(2^{\alpha}) - 3(4^{\alpha}) + 2]; & for\, d > 2\, and\, n = 2 \\ (2^{\alpha})dn + [1 - 3(2^{\alpha}) + 3^{\alpha} + 4^{\alpha}]d + [2(2^{\alpha}) \\ -3(4^{\alpha})]; & for\, d > 2\, and\, n > 2 \end{cases} $$

where $G_d(P_n, v)$ is a bridge molecular graph of path graph P_n with n vertices and α is any real number.

Proof. By analyzing the molecular structure of the line graph of bridge molecular graph $G_d(P_n, v)$ of path graph P_n with n vertices.

For $d = 2$ and $n \geq 2$: we infer $v_1 = 2$, $v_2 = 2n - 3$ and $v_3 = 0$. Therefore, using the definition of zeroth-order general Randić index, we obtain

$$ \begin{aligned} {}^{0}\mathrm{R}_{\alpha}(L(G_d(P_n,v))) &= \sum_{v \in V(L(G_d(P_n,v)))} [d(v)]^{\alpha} \\ &= \sum_{v \in V_1} (1)^{\alpha} + \sum_{v \in V_2} (2)^{\alpha} + \sum_{v \in V_3} (3)^{\alpha} \\ &= 1(2) + 2^{\alpha}(2n-3) + 3^{\alpha}(0) \\ &= 2(2^{\alpha})n - 3(2^{\alpha}) + 2. \end{aligned} $$

For $d > 2$ and $n = 2$: we infer $v_1 = 2$, $v_2 = d - 2$, $v_3 = 2$ and $v_4 = d - 3$. Therefore, using the definition of zeroth-order general Randić index, we obtain

$$ \begin{aligned} {}^{0}\mathrm{R}_{\alpha}(L(G_d(P_n,v))) &= \sum_{v \in V(L(G_d(P_n,v)))} [d(v)]^{\alpha} \\ &= \sum_{v \in V_1} (1)^{\alpha} + \sum_{v \in V_2} (2)^{\alpha} + \sum_{v \in V_3} (3)^{\alpha} + \sum_{v \in V_4} (4)^{\alpha} \\ &= 1(2) + 2^{\alpha}(d-2) + 3^{\alpha}(2) + 4^{\alpha}(d-3) \\ &= (2^{\alpha} + 4^{\alpha})d + [2(3^{\alpha}) - 2(2^{\alpha}) - 3(4^{\alpha}) + 2]. \end{aligned} $$

For $d > 2$ and $n > 2$: we infer $v_1 = d$, $v_2 = dn - 3d + 2$, $v_3 = d$ and $v_4 = d - 3$. Therefore, using the definition of zeroth-order general Randić index, we obtain

$$ \begin{aligned} {}^{0}\mathrm{R}_{\alpha}(L(G_d(P_n,v))) &= \sum_{v \in V(L(G_d(P_n,v)))} [d(v)]^{\alpha} \\ &= \sum_{v \in V_1} (1)^{\alpha} + \sum_{v \in V_2} (2)^{\alpha} + \sum_{v \in V_3} (3)^{\alpha} + \sum_{v \in V_4} (4)^{\alpha} \\ &= 1(d) + 2^{\alpha}(dn - 3d + 2) + 3^{\alpha}(d) + 4^{\alpha}(d-3) \\ &= (2^{\alpha})dn + [1 - 3(2^{\alpha}) + 3^{\alpha} + 4^{\alpha}]d + [2(2^{\alpha}) - 3(4^{\alpha})]. \end{aligned} $$

□

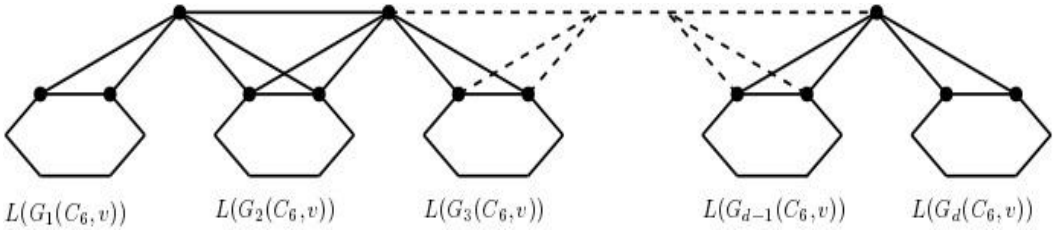

Fig. 5.2. Line graph of the bridge molecular graph $L(G_d(C_6, v))$.

Theorem 5.2. The zeroth-order general Randić index of line graph of $G_d(C_n, v)$ is:

$$ {}^{0}\mathrm{R}_{\alpha}\left(L(G_d(C_n,v))\right) = \begin{cases} 2(2^{\alpha})n + [4(3^{\alpha}) + 4^{\alpha} - 4(2^{\alpha})]; & for\, n > 2\, and\, d = 2 \\ (2^{\alpha})dn + [2(4^{\alpha}) - 2(2^{\alpha}) + 6^{\alpha}]d & \\ +[4(3^{\alpha}) - 4(4^{\alpha}) + 2(5^{\alpha}) - 3(6^{\alpha})]; & for\, n > 2\, and\, d > 2 \end{cases} $$

where $G_d(C_n, v)$ is a bridge molecular graph of cyclic graph C_n with n vertices and α is any real number.

Proof. Using the vertex dividing technique for the line graph of bridge molecular graph $G_d(C_n, v)$ of cyclic graph C_n with n vertices.

For $n > 2$ and $d = 2$: we infer $v_2 = 2n - 4$, $v_3 = 4$ and $v_4 = 1$. Therefore, using the definition of zeroth-order general Randić index, we obtain

$$\begin{aligned} {}^{0}\mathrm{R}_{\alpha}(L(G_d(C_n,v))) &= \sum_{v\in V(L(G_d(C_n,v)))} [d(v)]^{\alpha} \\ &= \sum_{v\in V_2} (2)^{\alpha} + \sum_{v\in V_3} (3)^{\alpha} + \sum_{v\in V_4} (4)^{\alpha} \\ &= 2^{\alpha}(2n-4) + 3^{\alpha}(4) + 4^{\alpha}(1) \\ &= 2(2^{\alpha})n + [4(3^{\alpha}) + 4^{\alpha} - 4(2^{\alpha})]. \end{aligned}$$

For $n > 2$ and $d > 2$: we infer $v_2 = dn - 2d$, $v_3 = 4$, $v_4 = 2d - 4$, $v_5 = 2$ and $v_6 = d - 3$. Therefore, using the definition of zeroth-order general Randić index, we obtain

$$\begin{aligned} {}^{0}\mathrm{R}_{\alpha}(L(G_d(C_n,v))) &= \sum_{v\in V(L(G_d(C_n,v)))} [d(v)]^{\alpha} \\ &= \sum_{v\in V_2} (2)^{\alpha} + \sum_{v\in V_3} (3)^{\alpha} + \sum_{v\in V_4} (4)^{\alpha} + \sum_{v\in V_5} (5)^{\alpha} + \sum_{v\in V_6} (6)^{\alpha} \\ &= 2^{\alpha}(dn-2d) + 3^{\alpha}(4) + 4^{\alpha}(2d-4) + 5^{\alpha}(2) + 6^{\alpha}(d-3) \\ &= (2^{\alpha})dn + [2(4^{\alpha}) - 2(2^{\alpha}) + 6^{\alpha}]d + [4(3^{\alpha}) - 4(4^{\alpha}) + 2(5^{\alpha}) - 3(6^{\alpha})]. \end{aligned}$$

□

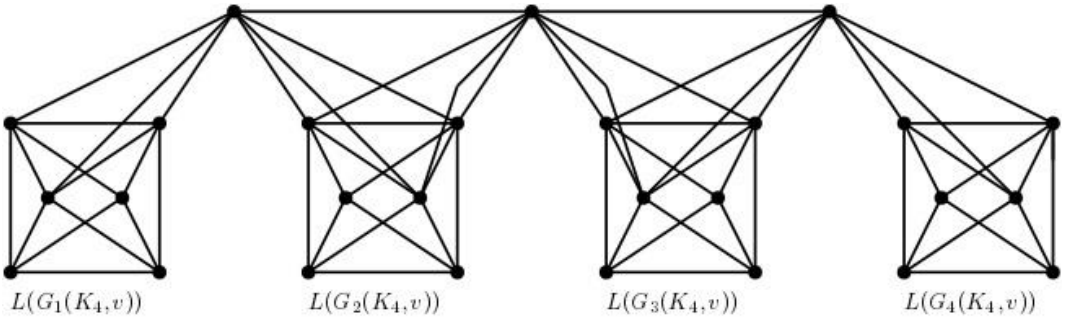

Fig. 5.3. Line graph of the bridge molecular graph $L(G_4(K_4, v))$.

Theorem 5.3. The zeroth-order general Randić index of line graph of $G_d(K_n, v)$ is:

$$
{}^{0}\mathrm{R}_{\alpha}\left(L(G_d(K_n,v))\right) = \begin{cases} 2(2^{\alpha})d + [2-3(2^{\alpha})]; & for\, n=2\, and\, d \geq 2 \\ (2n-4)^{\alpha}(n^2-3n+2) + (2n-3)^{\alpha} & \\ (2n-2) + (2n-2)^{\alpha}; & for\, n>2\, and\, d=2 \\ (2n-4)^{\alpha}(\frac{3}{2}n^2 - \frac{9}{2}n + 3) + (2n-3)^{\alpha} & \\ (2n-2) + (2n-2)^{\alpha}(n-1) + 2(2n-1)^{\alpha}; & for\, n>2\, and\, d=3 \\ (2n-4)^{\alpha}(\frac{1}{2}dn^2 - \frac{3}{2}dn + d) + (2n-3)^{\alpha} & \\ (2n-2) + (2n-2)^{\alpha}(dn-d-2n+2) & \\ +2(2n-1)^{\alpha} + (2n)^{\alpha}(d-3); & for\, n>2\, and\, d>3 \end{cases}
$$

where $G_d(K_n, v)$ is a bridge molecular graph of complete graph K_n with n vertices and α is any real number.

Proof. By analyzing the molecular structure of the line graph of bridge molecular graph $G_d(K_n, v)$ of complete graph K_n with n vertices.

For $n = 2$ and $d \geq 2$: we infer $v_1 = 2$ and $v_2 = 2d - 3$. Therefore, using the definition of zeroth-order general Randić index, we obtain

$$
\begin{aligned}
{}^{0}\mathrm{R}_{\alpha}(L(G_d(K_n,v))) &= \sum_{v \in V(L(G_d(K_n,v)))} [d(v)]^{\alpha} \\
&= \sum_{v \in V_1} (1)^{\alpha} + \sum_{v \in V_2} (2)^{\alpha} \\
&= 1(2) + 2^{\alpha}(2d-3) \\
&= 2(2^{\alpha})d + [2-3(2^{\alpha})].
\end{aligned}
$$

For $n > 2$ and $d = 2$: we infer: $v_{2n-4} = n^2 - 3n + 2$, $v_{2n-3} = 2n - 2$ and $v_{2n-2} = 1$. Therefore, using the definition of zeroth-order general Randić index, we obtain

$$
\begin{aligned}
{}^{0}\mathrm{R}_{\alpha}(L(G_d(K_n,v))) &= \sum_{v\in V(L(G_d(K_n,v)))} [d(v)]^{\alpha} \\
&= \sum_{v\in V_{2n-4}} (2n-4)^{\alpha} + \sum_{v\in V_{2n-3}} (2n-3)^{\alpha} + \sum_{v\in V_{2n-2}} (2n-2)^{\alpha} \\
&= (2n-4)^{\alpha}(n^2-3n+2) + (2n-3)^{\alpha}(2n-2) + (2n-2)^{\alpha}.
\end{aligned}
$$

For $n > 2$ and $d = 3$: we infer: $v_{2n-4} = \frac{3}{2}(n^2 - 3n + 2)$, $v_{2n-3} = 2n - 2$, $v_{2n-2} = n - 1$ and $v_{2n-1} = 2$. Therefore, using the definition of zeroth-order general Randić index, we obtain

$$
\begin{aligned}
{}^{0}\mathrm{R}_{\alpha}(L(G_d(K_n,v))) &= \sum_{v\in V(L(G_d(K_n,v)))} [d(v)]^{\alpha} \\
&= \sum_{v\in V_{2n-4}} (2n-4)^{\alpha} + \sum_{v\in V_{2n-3}} (2n-3)^{\alpha} + \sum_{v\in V_{2n-2}} (2n-2)^{\alpha} + \sum_{v\in V_{2n-1}} (2n \\
&\quad -1)^{\alpha} \\
&= (2n-4)^{\alpha}\left(\frac{3}{2}n^2 - \frac{9}{2}n + 3\right) + (2n-3)^{\alpha}(2n-2) + (2n-2)^{\alpha}(n-1) + \\
&\quad 2(2n-1)^{\alpha}.
\end{aligned}
$$

For $n > 2$ and $d > 3$: we infer: $v_{2n-4} = \frac{d}{2}(n^2 - 3n + 2)$, $v_{2n-3} = 2n - 2$, $v_{2n-2} = dn - d - 2n + 2$, $v_{2n-1} = 2$ and $v_{2n} = d - 3$. Therefore, using the definition of zeroth-order general Randić index, we obtain

$$
\begin{aligned}
{}^{0}\mathrm{R}_{\alpha}(L(G_d(K_n,v))) &= \sum_{v\in V(L(G_d(K_n,v)))} [d(v)]^{\alpha} \\
&= \sum_{v\in V_{2n-4}} (2n-4)^{\alpha} + \sum_{v\in V_{2n-3}} (2n-3)^{\alpha} + \sum_{v\in V_{2n-2}} (2n-2)^{\alpha} + \sum_{v\in V_{2n-1}} (2n \\
&\quad -1)^{\alpha} + \sum_{v\in V_{2n}} (2n)^{\alpha} \\
&= (2n-4)^{\alpha}\left(\frac{1}{2}dn^2 - \frac{3}{2}dn + d\right) + (2n-3)^{\alpha}(2n-2) + (2n-2)^{\alpha}(dn-d \\
&\quad -2n+2) + 2(2n-1)^{\alpha} + (2n)^{\alpha}(d-3).
\end{aligned}
$$

□

7. Zeroth-order general Randić index of line graph of carbon tube network

The name carbon nanotube is derived from its long, cylindrical and hollow composition. Carbon nanotubes are allotropes of carbon. They have many

structures; differing in length, thickness, and number of layers. The properties of nanotubes can be different depending on how the graphene sheet has rolled up to form the tube causing it to act either metallic or as a semiconductor.

"Consider the *m* x *n* quadrilateral section P_m^n with $m \geq 2$ hexagons on the top and bottom sides and $n \geq 2$ hexagons on the lateral sides cut from the regular hexagonal lattice". See Bača et al. [2] for more details.

"If we identify two lateral sides of P_m^n such that we identify the vertices u_0^j and u_m^j for $j = 0, 1, 2, \ldots, n$, then we obtain the nanotube NA_m^n".

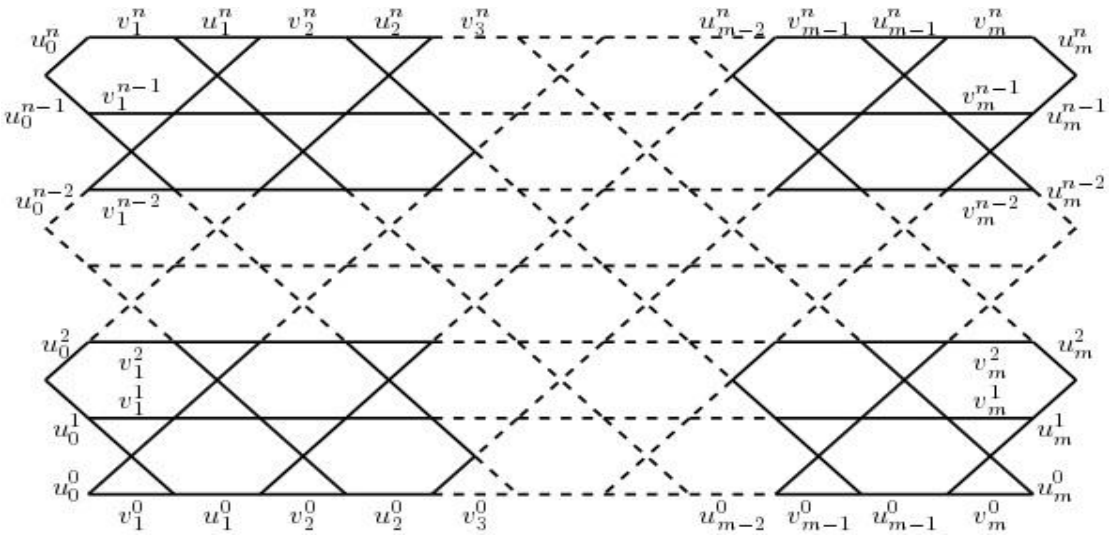

Fig. 6. Line graph of the quadrilateral section P_m^n cuts from the regular hexagonal lattice

Theorem 6.1. The zeroth-order general Randić index of line graph of NA_m^n is:

$$^0\mathrm{R}_\alpha(L(NA_m^n)) = [3(4^\alpha)]mn + 2[2(3^\alpha) - 4^\alpha]m.$$

where NA_m^n is a molecular graph of carbon nanotube for *m*, $n \geq 2$ and α is any real number.

Proof. For the line graph of tube NA_m^n: we derive $v_3 = 4m$ and $v_4 = 3mn - 2m$. Hence, by means of the definition of zeroth-order general Randić index, we get

$$
\begin{aligned}
{}^{0}\mathrm{R}_{\alpha}(L(NA_m^n)) &= \sum_{v\in V(L(NA_m^n))} [d(v)]^{\alpha} \\
&= \sum_{v\in V_3} (3)^{\alpha} + \sum_{v\in V_4} (4)^{\alpha} \\
&= 3^{\alpha}(4m) + 4^{\alpha}(3mn - 2m) \\
&= [3(4^{\alpha})]mn + 2[2(3^{\alpha}) - 4^{\alpha}]m.
\end{aligned}
$$

□

Let n be even, $n \geq 2$, and $m \geq 2$. "If we identify the top and bottom sides of the quadrilateral section P_m^n in such a way that we identify the vertices u_i^0 and u_i^n for $i = 0, 1, 2, \ldots, m$, and the vertices v_i^0 and v_i^n for $i = 1, 2, 3, \ldots, m$, then we obtain the carbon nanotube NC_m^n".

Theorem 6.2. The zeroth-order general Randić index of line graph of NC_m^n is:

$$
{}^{0}\mathrm{R}_{\alpha}(L(NC_m^n)) = \begin{cases} 3(4^{\alpha})mn + [2^{\alpha} + 2(3^{\alpha}) - \frac{5}{2}(4^{\alpha})]n; & for\ n \geq 2\ and\ n\ is\ even \\ 3(4^{\alpha})mn + [2^{\alpha} + 2(3^{\alpha}) - \frac{5}{2}(4^{\alpha})]n + [\frac{1}{2}(4^{\alpha}) - 2^{\alpha}]; & for\ n \geq 2\ and\ n\ is\ odd \end{cases}
$$

where NC_m^n is a molecular graph of carbon nanotube for $n \geq 2$ even and $m \geq 2$ and α is any real number.

Proof. For $n \geq 2$ and n is even: By means of structure analysis of the line graph of tube NC_m^n, we derive $v_2 = n$, $v_3 = 2n$ and $v_4 = 3mn - \frac{5}{2}n$. Hence, by using the definition of zeroth-order general Randić index, we get

$$
\begin{aligned}
{}^{0}\mathrm{R}_{\alpha}(L(NC_m^n)) &= \sum_{v\in V(L(NC_m^n))} [d(v)]^{\alpha} \\
&= \sum_{v\in V_2} (2)^{\alpha} + \sum_{v\in V_3} (3)^{\alpha} + \sum_{v\in V_4} (4)^{\alpha} \\
&= 2^{\alpha}(n) + 3^{\alpha}(2n) + 4^{\alpha}(3mn - \frac{5}{2}n) \\
&= 3(4^{\alpha})mn + [2^{\alpha} + 2(3^{\alpha}) - \frac{5}{2}(4^{\alpha})]n.
\end{aligned}
$$

For $n \geq 2$ and n is odd: By means of structure analysis of line graph of tube NC_m^n, we derive $v_2 = n - 1$, $v_3 = 2n$ and $v_4 = 3mn - \frac{5}{2}n + \frac{1}{2}$. Hence, by using the definition of zeroth-order general Randić index, we get

$$
\begin{aligned}
{}^{0}\mathrm{R}_{\alpha}(L(NC_m^n)) &= \sum_{v\in V(L(NC_m^n))} [d(v)]^{\alpha} \\
&= \sum_{v\in V_2} (2)^{\alpha} + \sum_{v\in V_3} (3)^{\alpha} + \sum_{v\in V_4} (4)^{\alpha} \\
&= 2^{\alpha}(n-1) + 3^{\alpha}(2n) + 4^{\alpha}(3mn - \frac{5}{2}n + \frac{1}{2}) \\
&= 3(4^{\alpha})mn + [2^{\alpha} + 2(3^{\alpha}) - \frac{5}{2}(4^{\alpha})]n + [\frac{1}{2}(4^{\alpha}) - 2^{\alpha}].
\end{aligned}
$$

□

8. Zeroth-order general Randić index of line graph of dendrimer stars $D_3[n]$

Dendrimers are nano-sized, radially symmetric molecules with well-defined chemical structure consisting of tree-like arms or branches. The structure of dendrimer molecules begins with a central atom or group of atoms labeled as the core. From this central structure, the branches of other atoms called dendrons grow through a variety of chemical reactions. In this section, we analyze an essential chemical structure $D_3[n]$ which denoted the n-th growth of star dendrimer for $\forall n \in \mathbb{N} \cup \{0\}$. For more details on the structure of this chemical molecular graph which is quite common in drug structures see Farahani [6].

Theorem 7. The zeroth-order general Randić index of line graph of $D_3[n]$ is:

$$
{}^{0}\mathrm{R}_{\alpha}(L(D_3[n])) = [15(2^{\alpha}) + 24(3^{\alpha}) + 9(4^{\alpha})]2^n - 6[2^{\alpha} + 2(3^{\alpha}) + 4^{\alpha}].
$$

where $D_3[n]$ is a molecular graph of the dendrimer stars having nth growth and α is any real number.

Proof. By observing the structure of line graph of dendrimer stars $D_3[n]$, we deduce its vertex partition with respect to the degrees as: $v_2 = 15(2^n) - 6$, $v_3 = 12(2^{n+1} - 1)$ and $v_4 = 9(2^n - 1) + 3$. Therefore, according to the definition of zeroth-order general Randić index, we check

$$
\begin{aligned}
{}^{0}\mathrm{R}_{\alpha}(L(D_3[n])) &= \sum_{v\in V(L(D_3[n]))} [d(v)]^{\alpha} \\
&= \sum_{v\in V_2} (2)^{\alpha} + \sum_{v\in V_3} (3)^{\alpha} + \sum_{v\in V_4} (4)^{\alpha} \\
&= 2^{\alpha}[15(2^{n}) - 6] + 3^{\alpha}[12(2^{n+1} - 1)] + 4^{\alpha}[9(2^{n}) - 6] \\
&= [15(2^{\alpha}) + 24(3^{\alpha}) + 9(4^{\alpha})]2^{n} - 6[2^{\alpha} + 2(3^{\alpha}) + 4^{\alpha}].
\end{aligned}
$$

□

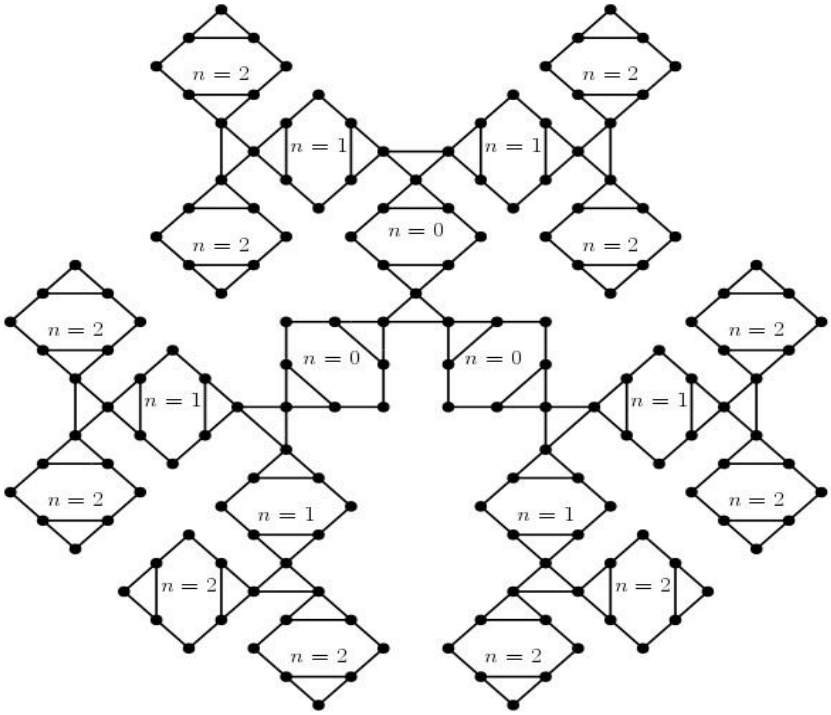

Fig. 7. 2-Dimensional line graph of the *n*th growth of star dendrimer $L(D_3[2])$

9. Zeroth-order general Randić index of line graph of circumcoronene series of benzenoid H_k

A benzenoid system is a connected collection of congruent regular hexagons arranged in a plane in such a way that two hexagons are either completely disjoint or have one common edge. The Circumcoronene Homologous Series of Benzenoid is a connected family of molecular graphs and has remarkable structure. This family generates from several copies of benzene C_6.

We denote the k-th terms of this series by H_k for $k \geq 1$. The first terms of this series are H_1 = benzene, H_2 = coronene, H_3 = circumcoronene, H_4 = circumcircumcoronene. See Farahani [7] for more structural details.

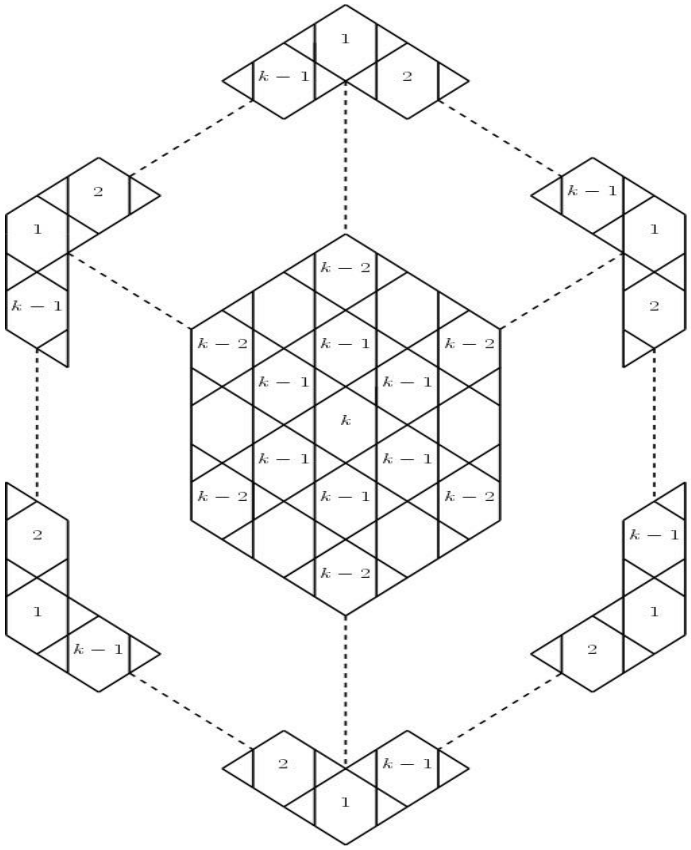

Fig. 8. Line graph of the circumcoronene series of benzenoid $L(H_k)$ for $k \geq 1$

Theorem 8. The zeroth-order general Randić index of line graph of H_k is:

$$^{0}\mathrm{R}_{\alpha}(L(H_k)) = [9(4^{\alpha})]k^2 + [12(3^{\alpha}) - 15(4^{\alpha})]k + [6(2^{\alpha}) - 12(3^{\alpha}) + 6(4^{\alpha})].$$

where H_k is a molecular graph of the circumcoronene series of benzenoid for $k \geq 1$ and α is any real number.

Proof. Consider the line graph of circumcoronene series of benzenoid H_k for $k \geq 1$. We deduce $v_2 = 6$, $v_3 = 12k - 12$ and $v_4 = 9k^2 - 15k + 6$. Thus, using the definition of zeroth-order general Randić index, we infer

$$
\begin{aligned}
{}^{0}\mathrm{R}_{\alpha}(L(H_k)) &= \sum_{v\in V(L(H_k))} [d(v)]^{\alpha} \\
&= \sum_{v\in V_2} (2)^{\alpha} + \sum_{v\in V_3} (3)^{\alpha} + \sum_{v\in V_4} (4)^{\alpha} \\
&= 2^{\alpha}(6) + 3^{\alpha}(12k-12) + 4^{\alpha}(9k^2-15k+6) \\
&= [9(4^{\alpha})]k^2 + [12(3^{\alpha}) - 15(4^{\alpha})]k + [6(2^{\alpha}) - 12(3^{\alpha}) + 6(4^{\alpha})].
\end{aligned}
$$

10. Zeroth-order general Randić index of line graph of capra-designed planar benzenoid series

Capra-designed planar benzenoid has symmetric structure. Capra *Ca* map operation enables one to build a new structure of a planar graph *G*. It is a method of drawing and modifying the covering of a polyhedral structure. Capra-operation of arbitrary graph *G* is *Ca*(*G*), iteration of Capra will be denoted by *CaCa*(*G*) (or we denote $Ca_2(G)$). By iterating the Capra-operation on the hexagon (i.e. benzene graph C_6) and its *Ca*-transforms, a benzenoid series can be designed. The first members of this series are denoted as *Ca*(C_6), $Ca_2(C_6)$ and $Ca_3(C_6)$. For more details regarding to the definition of Capra-transform, and the structure of Capra-designed planar benzenoid series, see Farahani and Vlad [8] and [9].

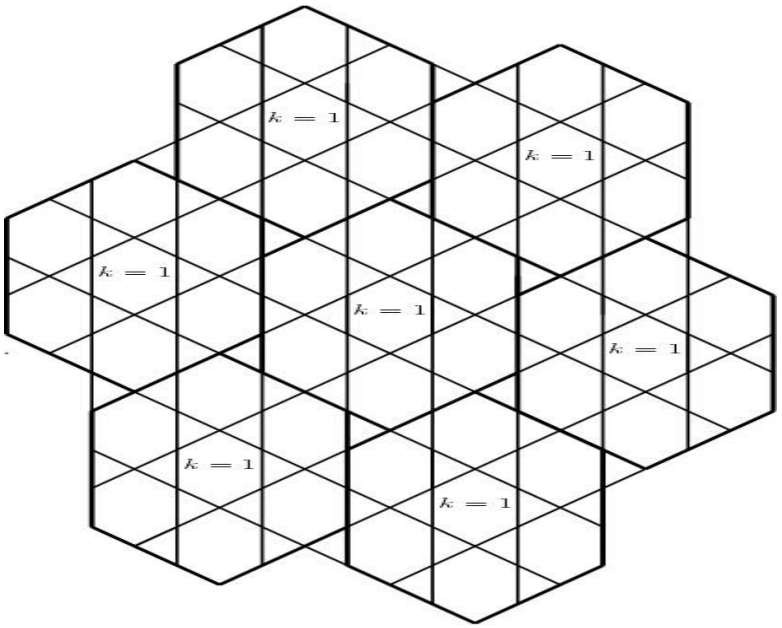

Fig. 9. Line graph of the capra-designed planar benzenoid series $L(Ca_2(C_6))$

Theorem 9. The zeroth-order general Randić index of line graph of $Ca_k(C_6)$ is:

$${}^{0}\mathrm{R}_{\alpha}(L(Ca_k(C_6))) = [3(4^{\alpha})]7^k + [4(3^{\alpha}) - 4^{\alpha}]3^k + 6(2^{\alpha} - 4^{\alpha})k^2 + 12(4^{\alpha} - 2^{\alpha})k + 12(2^{\alpha} - 4^{\alpha}).$$

where $Ca_k(C_6)$ is a molecular graph of the capra-designed planar benzenoid series and α is any real number.

Proof. By analyzing the molecular structure of line graph of $Ca_k(C_6)$, we check that the vertex set of line graph of $Ca_k(C_6)$ can be divided into three partitions: $v_2 = 6k^2 - 12k + 12$, $v_3 = 12(3^{k-1})$ and $v_4 = 3(7^k) - 1(3^k) - 6k^2 + 12k - 12$. Thus, using the definition of zeroth-order general Randić index, we infer

$$\begin{aligned}
{}^{0}\mathrm{R}_{\alpha}(L(Ca_k(C_6))) &= \sum_{v \in V(L(Ca_k(C_6)))} [d(v)]^{\alpha} \\
&= \sum_{v \in V_2} (2)^{\alpha} + \sum_{v \in V_3} (3)^{\alpha} + \sum_{v \in V_4} (4)^{\alpha} \\
&= 2^{\alpha}(6k^2 - 12k + 12) + 3^{\alpha}[12(3^{k-1})] + 4^{\alpha}[3(7^k) - 1(3^k) - 6k^2 + 12k - 12] \\
&= [3(4^{\alpha})]7^k + [4(3^{\alpha}) - 4^{\alpha}]3^k + 6(2^{\alpha} - 4^{\alpha})k^2 + 12(4^{\alpha} - 2^{\alpha})k + 12(2^{\alpha} - 4^{\alpha}).
\end{aligned}$$

□

11. Conclusions

Recent endeavors in field of molecular topology shed light on unprecedented use of topological indices in rectifying the viral diseases that is valuable for pharmaceutical and medical scientists to comprehend the biological and chemical characteristics of new drugs. We have derived general formulas for calculating the zeroth-order general Randić index of line graphs of various well-known chemical structures, see Theorems 1-9. These theorems may be useful for predicting and theoretically identify certain physiochemical properties of drug molecular structures including boiling point, degree of branching, etc. of the considered chemical structures [15, 16].

Acknowledgement

The authors would like to thank both the reviewers for their kind comments and valuable suggestions, which improved the paper considerably.

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