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FORGOTTEN TOPOLOGICAL INDEX OF LINE GRAPHS OF SOME CHEMICAL STRUCTURES IN DRUGS

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Abstract: A large number of drug experiments revealed that there exists strong inherent relation between the drugs molecular structures and the bio-medical and pharmacology characteristics. Due to the effectiveness for pharmaceutical and medical scientists of their ability to grasp the biological and chemical characteristics of new drugs, forgotten topological index was defined to analyze the drug molecular structures. This index is applicable for testing the chemical and pharmacological properties of drug molecular structures that can make up for lack of chemical experiments and can provide a theoretical basis for the manufacturing of drugs which is widely welcomed in developing areas. In this paper, based on the drug molecular structure analysis and vertex dividing technique with respect to their degrees, we present the forgotten topological index of the line graphs of several popular chemical structures which is quite common in drug molecular graphs.

Keywords: Computational medical, Forgotten topological index, Line graphs, Dendrimer stars, Bridge graph, Benzenoid series.

Introduction

In this era of rapid technological development of medicine manufacture, chemical and pharmaceutical techniques have been promptly

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evolved, and thus a large number of new nano-materials, crystalline materials, and drugs emerge every year. A tremendous amount of chemical experiments and work is required to determine the chemical properties of new compounds and drugs to test their physical, chemical and biological properties. Sufficient equipment, reagents and human resources are required to investigate the performance and the side effects of existing new drugs. However, in poor background areas and in developing countries (like some countries in Southeast Asia, South America and Africa) there are inadequate money and funds to afford such equipment and reagents which can be used to measure their biochemical and pharmaceutical properties.

Numerous previous studies and the chemical based experiments have revealed that there exists strong correspondence between molecular structures and their physical behaviors, chemical characteristics, and biological features, such as melting point, boiling point, and toxicity of drugs. If we enumerate indicators of these drug molecular structures in accordance with the topological indices, the medical and pharmaceutical researchers could find it beneficial to well know their medicinal properties, which can make up the defects of medicine and chemical experiments. From this perspective, we can appreciate the effectiveness of the methods on the topological index of computation especially for developing countries, 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 hardware.

Conventionally in medicine mathematical model, the structure of a drug is considered as an undirected 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)*. 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. Scientists have introduced significant indices decades ago, including Wiener index, PI index, Zagreb index and eccentric index, to measure the characteristics of the drug molecules. Several reports help to determine these topological indices of special molecular graphs in chemical, nano-materials and pharmaceutical engineering. See Refs. [1,2,3,4,5,6,7,8] for more details. In this paper, the referred notations and terminologies without clear explanation can be found in Bondy and Mutry.[9]

Results and Discussion

Since the 1970s, two degree based graph invariants have been extensively studied. These are the first Zagreb index M_1 and the second Zagreb index M_2. The Zagreb index M_1 was first time encountered in a paper published in 1972, where a series of approximate formulas for total π-electron energy ϵ were deduced. By means of these formulas, several structural details have been identified, on which ϵ depends. In the paper presented by Gutman and Trinajstic,[10] in the same approximate formulas for ϵ, there was also a term equal to the sum of cubes of the vertex degrees of the molecular graph. For reasons not easy to comprehend, this latter term did not attract any attention, and in the next more than 40 years was completely ignored by scholars doing research on degree based topological indices.[11] In a recent article by Furtula and Gutman,[12] where they reinvestigated this index and studied some of its fundamental properties. They showed this index can enhance the physico-chemical capability of Zagreb index.

Followed by the first and second Zagreb indices, Furtula and Gutman[12] introduced forgotten topological index (also called *F*-index) which was defined as:

$$F(G) = \sum_{v \in V(G)} d(v)^3 = \sum_{uv \in E(G)} [d(u)^2 + d(v)^2],$$

where $d(v)$ is denoted as the degree of vertex v (the number of vertex adjacent to vertex v). It was discovered that forgotten topological index has some outstanding applications or unexpected mathematical properties. The linear combination $M_1 + F$ yields a highly accurate mathematical model of certain physico-chemical properties of alkanes.[13] Furtula and Gutman[12] analyze that the predictive ability of forgotten topological index is almost similar to that of first Zagreb index and for the acentric factor and entropy, and both of them obtain correlation coefficients larger than 0.95. This success encouraged researchers to search for mathematical properties of the *F*-index. This index is applicable for testing the chemical and pharmacological properties of drug molecular structures.

Even though there have been a lot of contributions on distance-based indices and degree-based molecular structures, the researches of forgotten topological index for some special drug structures are still largely limited. Due to this, enormous academic and industrial interest has been captivated to research *F*-index of drug molecular structure from a mathematical point of view.

Let $\delta(G)$ and $\Delta(G)$ be the minimum and maximum degree of G, respectively. 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, Siddiqui, Imran, Jamil and Farahani[2] we obtained the forgotten topological index of line graphs of several important chemical structures in drugs.

(i) Forgotten topological index of line graph of graphene *G*(*m, n*)

Graphene is a two-dimensional layer of pure carbon. It is a one-atom-thick and single tightly packed layer of carbon atoms that are bonded together in a repeating pattern of hexagons, with each carbon atom covalently bonded to three other carbon atoms. It is the building-block of Graphite. Graphene, unlike a buckyball or nanotube, has no inside because it is at. 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. See Shigehalli and Kanabur[14] for more details. Line graph of graphene *G*(*m,n*) is shown below in figure 1.

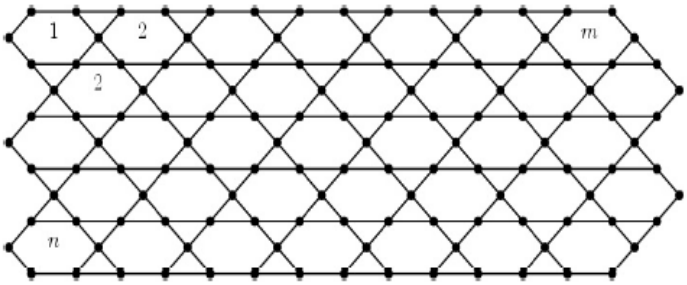

Figure 1. 2-Dimensional line graph of graphene sheet.

Theorem 1. The forgotten topological index of line graph of *G*(*m, n*) is:

$$F\left(L\left(G(m,n)\right)\right) = \begin{cases} 172m - 124; & for\ n = 1 \\ 192mn - 20m - 2n - 140; & for\ n \geq 2 \end{cases}$$

where *G*(*m, n*) is a molecular graph of graphene with *n* rows and *m* columns.

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 forgotten topological index, we obtain

$$F\left(L\left(G(m,n)\right)\right) = \sum_{v \in V\left(L\left(G(m,n)\right)\right)} d(v)^3$$

$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$

$$= 8(6) + 27(4m - 4) + 64(m - 1)$$

$$= 172m - 124.$$

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 forgotten topological index, we obtain

$$F\left(L\left(G(m,n)\right)\right) = \sum_{v \in V\left(L\left(G(m,n)\right)\right)} d(v)^3$$

$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$

$$= 8(n + 4) + 27(4m + 2n - 4) + 64(3mn - 2m - n - 1)$$

$$= 192mn - 20m - 2n - 140.$$

(ii) Forgotten topological index of line graph of three family of dendrimer stars

The nanostar dendrimers are part of a new group of macromolecules that appear to be photon funnels. The nanostar dendrimers are hyper-branched nanostructures that can be synthesized by divergent or convergent methods, and they are built up from branched units called monomers using a nanoscale fabrication process. In this section, we determine the line graph of three famous infinite classes $NS_1[n]$, $NS_2[n]$ and $NS_3[n]$ (figures 2.1, 2.2 and 2.3) of dendrimer stars which widely appear in the drug structures. For detailed structure, see Ashrafi and Nikzad.[15,24]

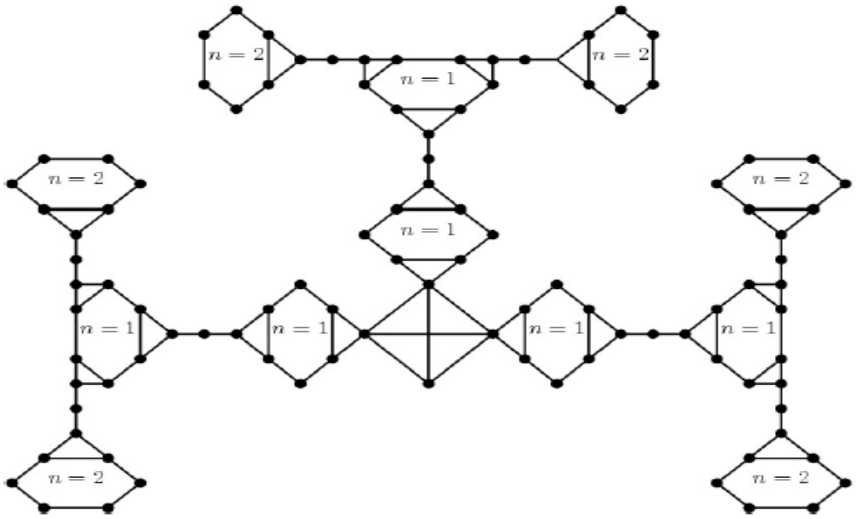

Figure 2.1. Line graph of the first type of nanostar dendrimer $L(NS_1[2])$.

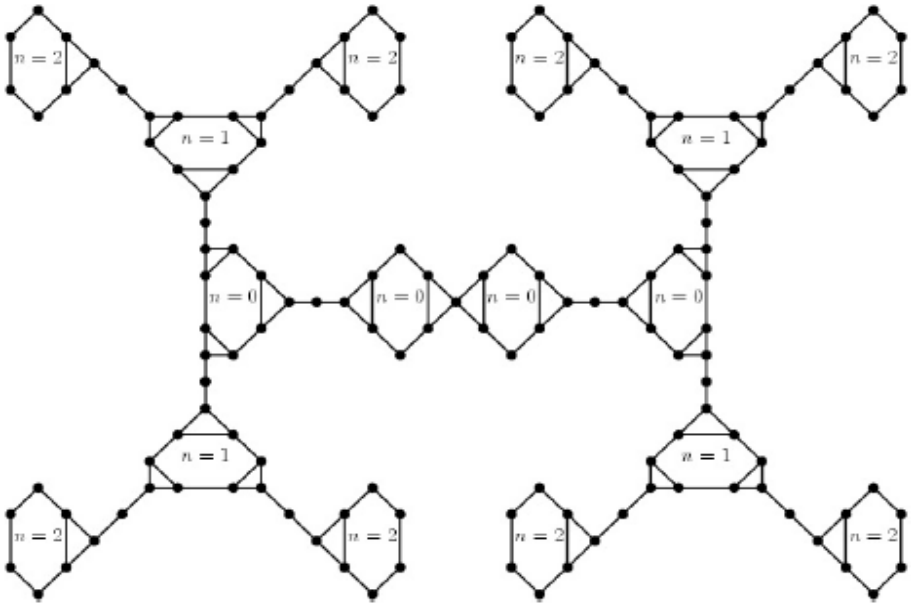

Figure 2.2. Line graph of the second type of nanostar dendrimer $L(NS_2[2])$.

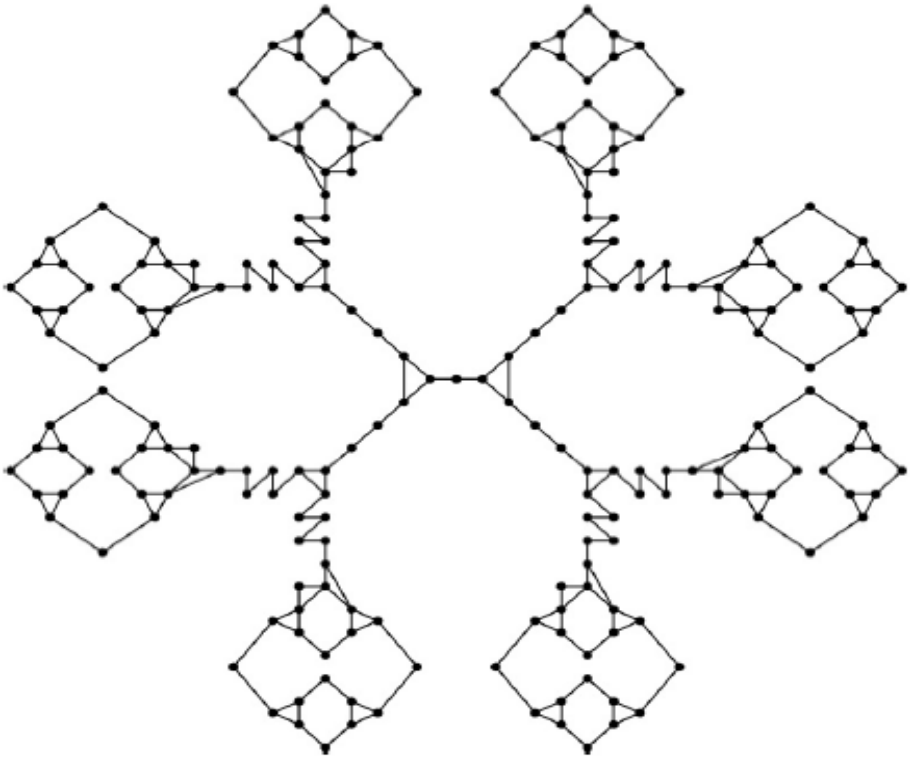

Figure 2.3. Line graph of the third type of nanostar dendrimer $L(NS_3[2])$.

Theorem 2. The forgotten topological index of line graphs of three infinite classes $NS_1[n]$, $NS_2[n]$ and $NS_3[n]$ of dendrimer stars is:

$$F\big(L(NS_1[n])\big) = 558(2^n) + 102$$

$$F\big(L(NS_2[n])\big) = 744(2^n) - 136$$

$$F\big(L(NS_3[n])\big) = 1332(2^n) - 218$$

where n is the number of steps of growth of these three family of dendrimer stars.

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 forgotten topological index, we check

$$F\big(L(NS_1[n])\big) = \sum_{v \in V\left(L(NS_1[n])\right)} d(v)^3$$

$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_5} (5)^3$$

$$= 8[9(2^n) + 3] + 27[18(2^n) - 11] + 125(3)$$

$$= 558(2^n) + 102.$$

$$F\big(L(NS_2[n])\big) = \sum_{v \in V\left(L(NS_2[n])\right)} d(v)^3$$

$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$

$$= 8[12(2^n - 1) + 14] + 27[24(2^n - 1) + 16] + 64(1)$$

$$= 744(2^n) - 136.$$

$$F\big(L(NS_3[n])\big) = \sum_{v \in V\left(L(NS_3[n])\right)} d(v)^3$$

$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$

$$= 8[48(2^{n-1} - 1) + 41] + 27[56(2^{n-1} - 1) + 50] + 64[12(2^{n-1})]$$

$$= 1332(2^n) - 218.$$

(iii) Forgotten topological 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. For the origin of polyominoes and more details can be found in the Refs. [16,17,18,25]. Line graph of polyomino chains of 8-cycles is shown in figure 3.

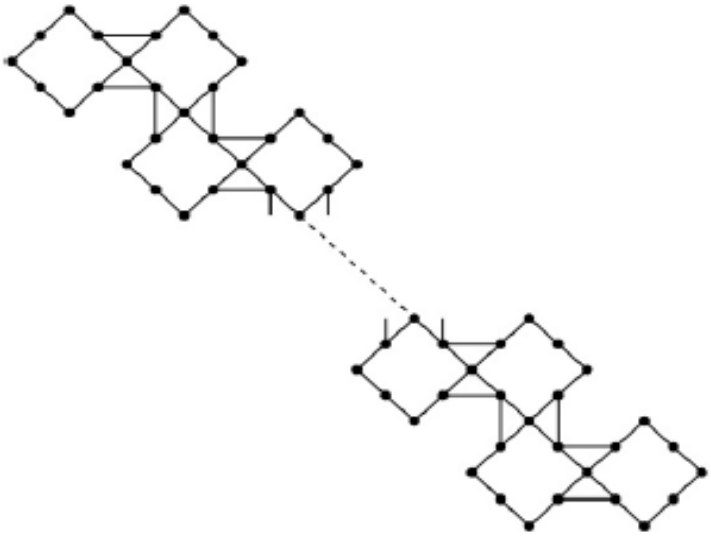

Figure 3. Line graph of the zig-zag chain of 8-cycles.

Theorem 3. The forgotten topological index of line graph of polyomino chain of 8-cycles is:

$$F\big(L(G)\big) = 824n - 160.$$

where *G* is a molecular graph of the zig-zag chain of 8-cycles.

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 forgotten topological index, we obtain

$$F(L(G)) = \sum_{v \in V(L(G))} d(v)^3$$

$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$

$$= 8(12n + 4) + 27(8n) + 64(8n - 3)$$

$$= 824n - 160.$$

(iv) Forgotten topological index of line graph of triangular benzenoid

Triangular benzenoid denoted by $T(n)$ is a family of benzenoid molecular graphs, which is the generalizations 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.[17] Line graph of triangular benzenoid is shown in figure 4.

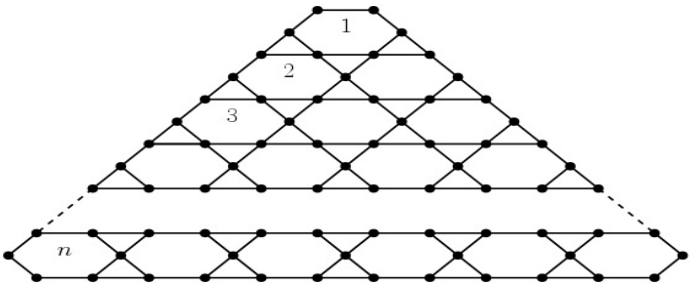

Figure 4. Line graph of triangular benzenoid $L(T(n))$.

Theorem 4. The forgotten topological index of line graph of $T(n)$ is:

$$F\big(L(T(n))\big) = 96n^2 + 66n - 114.$$

where $T(n)$ is a molecular graph of triangular benzenoid.

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 forgotten topological index, we get

$$F(L(T(n))) = \sum_{v \in V(L(T(n)))} d(v)^3$$

$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$

$$= 8(6) + 27[6(n-1)] + 64[\frac{3}{2}(n^2 - n)]$$

$$= 96n^2 + 66n - 114.$$

(v) Forgotten topological 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 $\{G_i\}_{i=1}^{d}$ regarding 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 linked 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 $G_1, \ldots, G_d$. Then we determine $L(G_d(H, v)) = L(B(H, \ldots, H; v, \ldots, v))$ for special situations 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 (See figures 5.1, 5.2 and 5.3), respectively. See Refs. [2,3] for more structural details.

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

Theorem 5.1. The forgotten topological index of line graph of $G_d(P_n, v)$ is:

$$F\left(L\left(G_d(P_n, v)\right)\right) = \begin{cases} 16n - 22; & for\ d = 2\ and\ n \geq 2 \\ 72d - 152; & for\ d > 2\ and\ n = 2 \\ 8dn + 68d - 176; & for\ d > 2\ and\ n > 2 \end{cases}$$

where $G_d(P_n, v)$ is a bridge molecular graph of path graph P_n with n vertices.

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 forgotten topological index, we obtain

$$F(L(G_d(P_n, v))) = \sum_{v \in V\left(L(G_d(P_n, v))\right)} d(v)^3$$

$$= \sum_{v \in V_1} (1)^3 + \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3$$

$$= 1(2) + 8(2n - 3) + 27(0)$$

$$= 16n - 22.$$

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 forgotten topological index, we obtain

$$F(L(G_d(P_n, v))) = \sum_{v \in V\left(L(G_d(P_n, v))\right)} d(v)^3$$

$$= \sum_{v \in V_1} (1)^3 + \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$

$$= 1(2) + 8(d - 2) + 27(2) + 64(d - 3)$$

$$= 72d - 152.$$

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 forgotten topological index, we obtain

$$F(L(G_d(P_n, v))) = \sum_{v \in V(L(G_d(P_n,v)))} d(v)^3$$
$$= \sum_{v \in V_1} (1)^3 + \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$
$$= 1(d) + 8(dn - 3d + 2) + 27(d) + 64(d - 3)$$
$$= 8dn + 68d - 176.$$

Theorem 5.2. The forgotten topological index of line graph of $G_d(C_n, v)$ is:

$$F\left(L\left(G_d(C_n, v)\right)\right) = \begin{cases} 16n + 140; & for\ n > 2\ and\ d = 2 \\ 8dn + 328d - 546; & for\ n > 2\ and\ d > 2 \end{cases}$$

where $G_d(C_n, v)$ is a bridge molecular graph of cyclic graph C_n with n vertices.

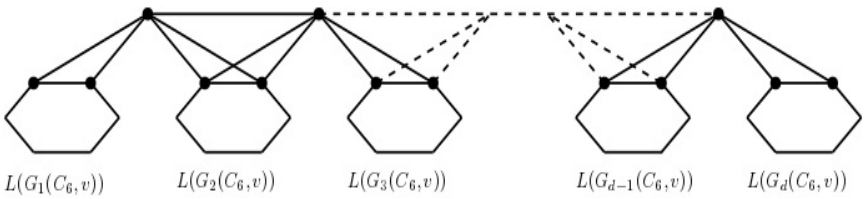

Figure 5.2. Line graph of the bridge molecular graph $L(G_d(C_6, v))$.

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 forgotten topological index, we obtain

$$F(L(G_d(C_n, v))) = \sum_{v \in V(L(G_d(C_n,v)))} d(v)^3$$
$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$
$$= 8(2n - 4) + 27(4) + 64(1)$$
$$= 16n + 140.$$

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 forgotten topological index, we obtain

$$F(L(G_d(C_n, v))) = \sum_{v \in V(L(G_d(C_n,v)))} d(v)^3$$
$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3 + \sum_{v \in V_5} (5)^3 + \sum_{v \in V_6} (6)^3$$
$$= 8(dn - 2d) + 27(4) + 64(2d - 4) + 125(2) + 216(d - 3)$$
$$= 8dn + 328d - 546.$$

Theorem 5.3. The forgotten topological index of line graph of $G_d(K_n, v)$ is:

$$F\left(L\left(G_d(K_n, v)\right)\right)$$
$$= \begin{cases} 16d - 22; & for\ n = 2\ and\ d \geq 2 \\ 8n^5 - 56n^4 + 176n^3 - 292n^2 + 246n - 82; & for\ n > 2\ and\ d = 2 \\ 12n^5 - 84n^4 + 280n^3 - 468n^2 + 394n - 132; & for\ n > 2\ and\ d = 3 \\ 4d(n^5 - 7n^4 + 26n^3 - 44n^2 + 40n - 14) - 2(16n^3 - 30n^2 + 43n - 18); & \\ & for\ n > 2\ and\ d > 3 \end{cases}$$

where $G_d(K_n, v)$ is a bridge molecular graph of complete graph K_n with n vertices.

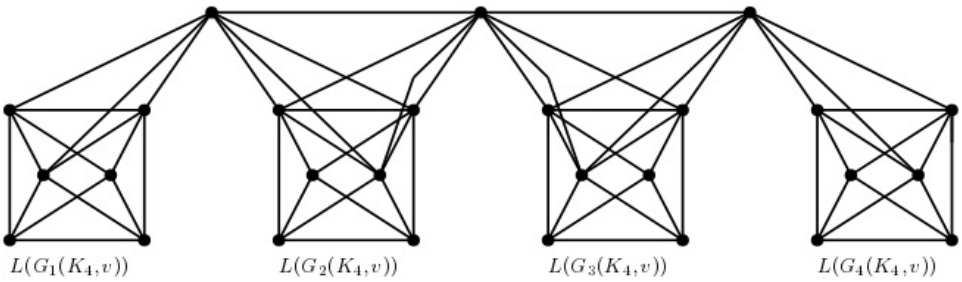

Figure 5.3. Line graph of the bridge molecular graph $L(G_4(K_4, v))$.

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 forgotten topological index, we obtain

$$F(L(G_d(K_n, v))) = \sum_{v \in V(L(G_d(K_n,v)))} d(v)^3$$
$$= \sum_{v \in V_1} (1)^3 + \sum_{v \in V_2} (2)^3$$
$$= 1(2) + 8(2d - 3)$$
$$= 16d - 22.$$

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 forgotten topological index, we obtain

$$F(L(G_d(K_n, v))) = \sum_{v \in V(L(G_d(K_n,v)))} d(v)^3$$
$$= \sum_{v \in V_{2n-4}} (2n-4)^3 + \sum_{v \in V_{2n-3}} (2n-3)^3 + \sum_{v \in V_{2n-2}} (2n-2)^3$$
$$= (8n^3 - 48n^2 + 96n - 64)(n^2 - 3n + 2) + (8n^3 - 36n^2 + 54n - 27)(2n - 2) + (8n^3 - 24n^2 + 24n - 8)(1)$$
$$= 8n^5 - 56n^4 + 176n^3 - 292n^2 + 246n - 82.$$

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 forgotten topological index, we obtain

$$F(L(G_d(K_n, v))) = \sum_{v \in V(L(G_d(K_n,v)))} d(v)^3$$
$$= \sum_{v \in V_{2n-4}} (2n-4)^3 + \sum_{v \in V_{2n-3}} (2n-3)^3 + \sum_{v \in V_{2n-2}} (2n-2)^3 + \sum_{v \in V_{2n-1}} (2n-1)^3$$

$$= (8n^3 - 48n^2 + 96n - 64)\left[\frac{3}{2}(n^2 - 3n + 2)\right] + (8n^3 - 36n^2 + 54n - 27)(2n - 2) + (8n^3 - 24n^2 + 24n - 8)(n - 1) + (8n^3 - 12n^2 + 6n - 1)(2) = 12n^5 - 84n^4 + 280n^3 - 468n^2 + 394n - 132.$$

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 forgotten topological index, we obtain

$$F(L(G_d(K_n, v))) = \sum_{v \in V(L(G_d(K_n,v)))} d(v)^3$$

$$= \sum_{v \in V_{2n-4}} (2n-4)^3 + \sum_{v \in V_{2n-3}} (2n-3)^3 + \sum_{v \in V_{2n-2}} (2n-2)^3 + \sum_{v \in V_{2n-1}} (2n-1)^3 + \sum_{v \in V_{2n}} (2n)^3$$

$$= (8n^3 - 48n^2 + 96n - 64)\left[\frac{d}{2}(n^2 - 3n + 2)\right] + (8n^3 - 36n^2 + 54n - 27)(2n - 2) + (8n^3 - 24n^2 + 24n - 8)(dn - d - 2n + 2) + (8n^3 - 12n^2 + 6n - 1)(2) + (8n^3)(d - 3)$$

$$= 4d(n^5 - 7n^4 + 26n^3 - 44n^2 + 40n - 14) - 2(16n^3 - 30n^2 + 43n - 18).$$

(vi) Forgotten topological index of line graph of carbon tube network

Carbon nanotubes are allotropes of carbon with a cylindrical nanostructure. Their name is derived from their long, hollow structure. These cylindrical carbon molecules have unusual properties that are important for nanotechnology, electronics, and other fields of materials science and technology. 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 Refs. [19] 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, …, n, then we obtain the nanotube NA_m^n. Line graph of the quadrilateral section P_m^n cuts from the regular hexagonal lattice is shown in figure 6.

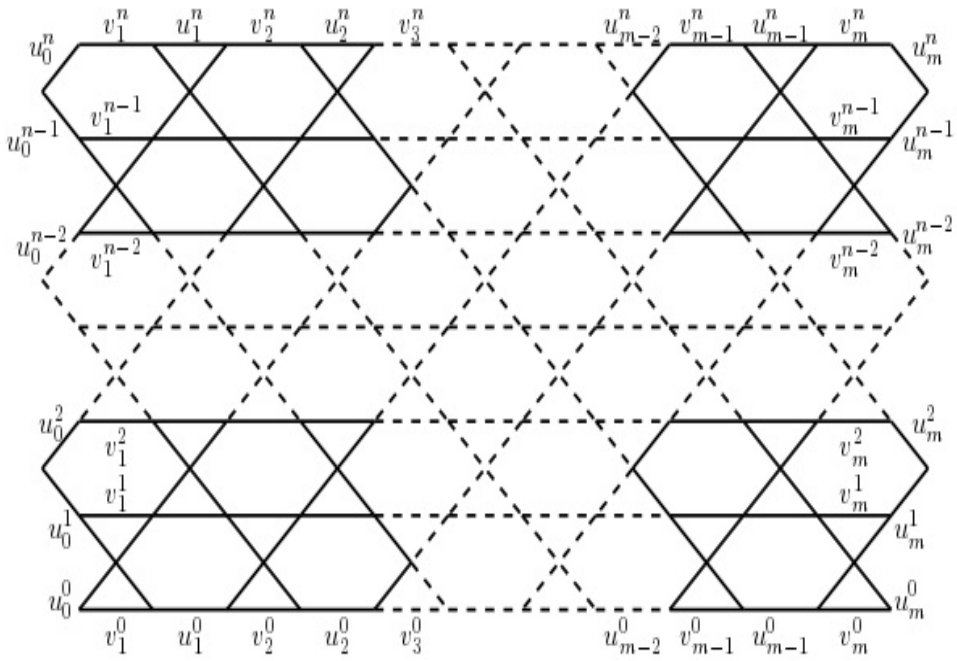

Figure 6. Line graph of the quadrilateral section P_m^n cuts from the regular hexagonal lattice.

Theorem 6.1. The forgotten topological index of line graph of NA_m^n is:

$$F\big(L(NA_m^n)\big) = 192mn - 20m.$$

where NA_m^n is a molecular graph of carbon nanotube for $m, n \geq 2$.

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 forgotten topological index, we get

$$F(L(NA_m^n)) = \sum_{v \in V(L(NA_m^n))} d(v)^3$$
$$= \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$
$$= 27(4m) + 64(3mn - 2m)$$
$$= 192mn - 20m.$$

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 forgotten topological index of line graph of NC_m^n is:

$$F\left(L(NC_m^n)\right) = \begin{cases} 192mn - 98n; & for\ n \geq 2\ and\ n\ is\ even \\ 192mn - 98n + 24; & for\ n \geq 2\ and\ n\ is\ odd \end{cases}$$

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

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 forgotten topological index, we get

$$F(L(NC_m^n)) = \sum_{v \in V(L(NC_m^n))} d(v)^3$$
$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$
$$= 8(n) + 27(2n) + 64(3mn - \frac{5}{2}n)$$
$$= 192\,mn - 98n.$$

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 forgotten topological index, we get

$$F(L(NC_m^n)) = \sum_{v \in V(L(NC_m^n))} d(v)^3$$
$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$
$$= 8(n-1) + 27(2n) + 64(3mn - \frac{5}{2}n + \frac{1}{2})$$
$$= 192mn - 98n + 24.$$

(vii) Forgotten topological index of line graph of dendrimer stars $D_3[n]$

Dendrimers have a very well-defined chemical structure with three major architectural components. These are the core, branches and end groups, where new branches are emitted from the core and are added in steps. In this section, an essential chemical structure $D_3[n]$ is analyzed. It describes the n-th growth of star dendrimer for $\forall n \in \mathrm{N} \cup \{0\}$. For more details on the structure of this chemical molecular graph which is quite common in drug structures see Farahani.[20] Line graph of the n-th growth of dendrimer star is shown in figure 7.

Theorem 7. The forgotten topological index of line graph of $D_3[n]$ is:

$$F\big(L(D_3[n])\big) = 1344(2^n) - 756.$$

where $D_3[n]$ is a molecular graph of the dendrimer stars having nth growth.

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 forgotten topological index, we check

$$F(L(D_3[n])) = \sum_{v \in V(L(D_3[n]))} d(v)^3$$

$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$
$$= 8[15(2^n) - 6] + 27[12(2^{n+1} - 1)] + 64[9(2^n - 1) + 3]$$
$$= 1344(2^n) - 756.$$

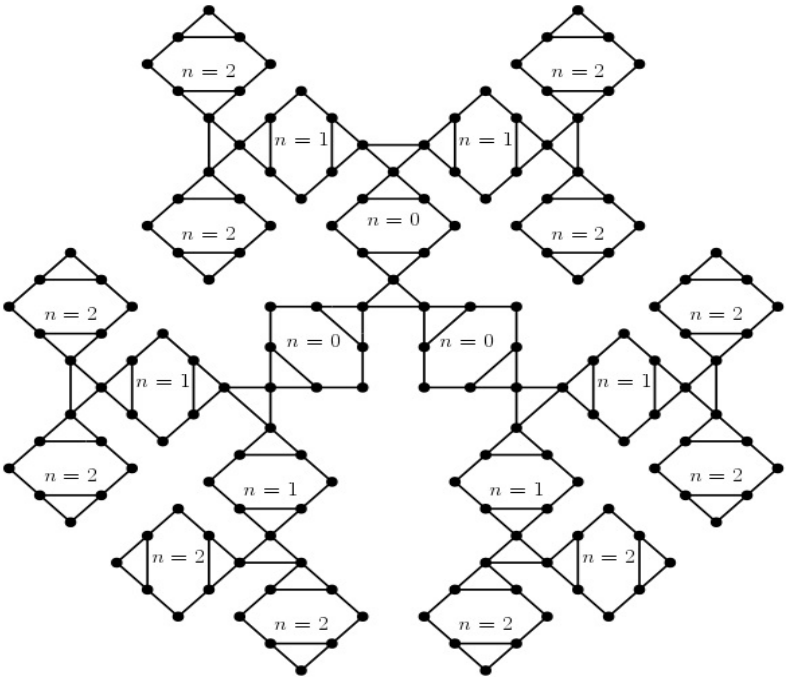

Figure 7. 2-Dimensional line graph of the *n*th growth of star dendrimer $L(D_3[2])$.

(viii) Forgotten topological index of line graph of circumcoronene series of benzenoid H_k

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 and benzene molecule is a usual molecule in chemistry, physics and nano-sciences. 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[21] for more structural details. Line graph of the circumcoronene series of benzenoid is shown in figure 8.

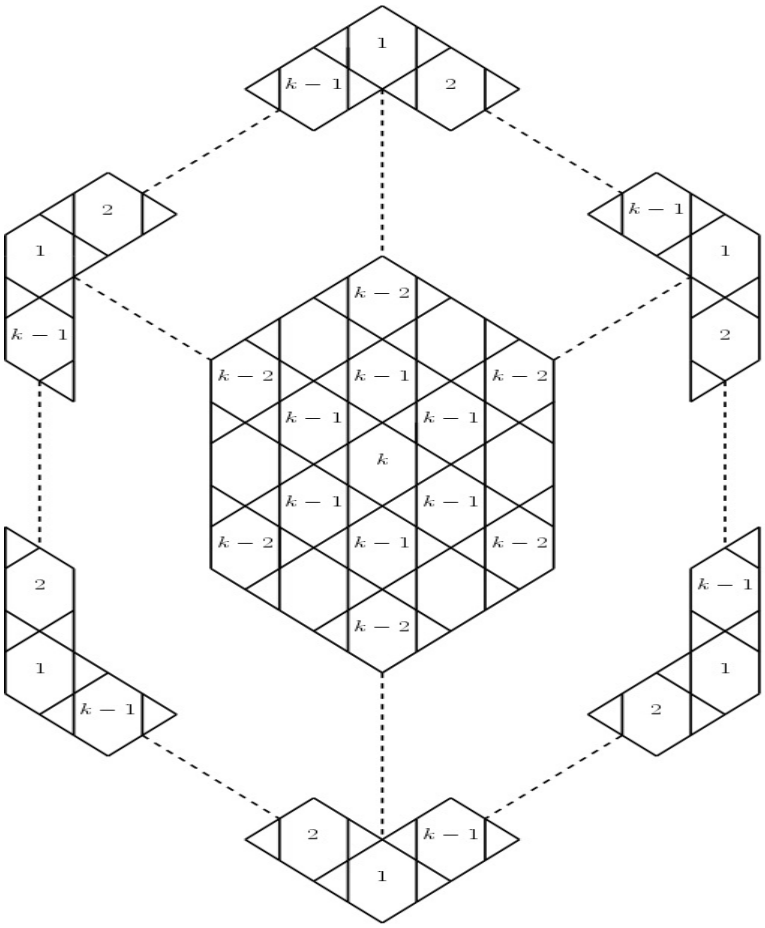

Figure 8. Line graph of the circumcoronene series of benzenoid $L(H_k)$ for $k \geq 1$.

Theorem 8. The forgotten topological index of line graph of H_k is:

$$F\big(L(H_k)\big) = 576(k^2) - 636(k) + 108.$$

where H_k is a molecular graph of the circumcoronene series of benzenoid for $k \geq 1$.

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 forgotten topological index, we infer

$$F(L(H_k)) = \sum_{v \in V(L(H_k))} d(v)^3$$
$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$
$$= 8(6) + 27(12k - 12) + 64(9k^2 - 15k + 6)$$
$$= 576k^2 - 636k + 108.$$

(ix) Forgotten topological index of line graph of capra-designed planar benzenoid series

Capra-designed planar benzenoid has symmetric structure. Capra *Ca* map operation 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. For more details regarding to the definition of Capra-transform and the structure of capra-designed planar benzenoid series see Farahani and Vlad.[22, 23] Line graph of the capra-designed planar benzenoid series is shown in figure 9.

Theorem 9. The forgotten topological index of line graph of $Ca_k(C_6)$ is:

$$F\big(L(Ca_k(C_6))\big) = 192(7^k) + 44(3^k) - 336(k^2) + 672(k - 1).$$

where $Ca_k(C_6)$ is a molecular graph of the capra-designed planar benzenoid series.

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 forgotten topological index, we infer

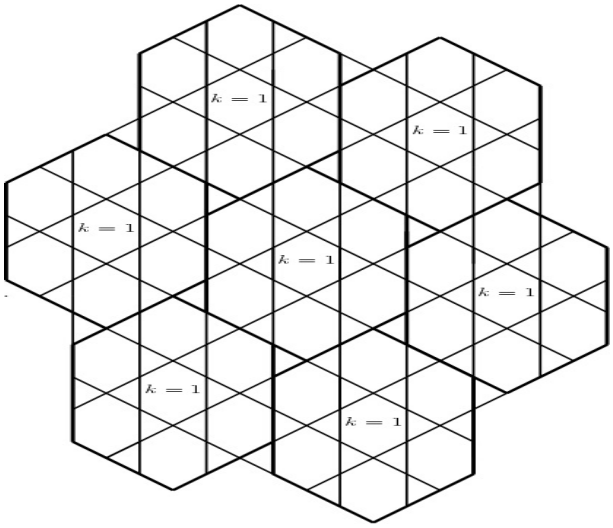

Figure 9. Line graph of the capra-designed planar benzenoid series $L(Ca_2(C_6))$.

$$F(L(Ca_k(C_6))) = \sum_{v \in V(L(Ca_k(C_6)))} d(v)^3$$

$$= \sum_{v \in V_2} (2)^3 + \sum_{v \in V_3} (3)^3 + \sum_{v \in V_4} (4)^3$$

$$= 8(6k^2 - 12k + 12) + 27[12(3^{k-1})] + 64[3(7^k) - 1(3^k) - -6k^2 + 12k - 12]$$

$$= 192(7^k) + 44(3^k) - 336(k^2) + 672(k - 1).$$

Conclusion

Every year a large number of new diseases are originated in the world, as a result of the contentiously emerging viruses at a high speed. Recent advances on the use of forgotten topological indices in rectifying the viral diseases are valuable for pharmaceutical and medical scientists to comprehend the biological and chemical characteristics of new drugs. This index is very suitable and serviceable for developing countries in which they can obtain the medical and biological information of new drugs without chemical experiment conditions. In this paper, in terms of drug

structure analysis and vertex dividing technique with respect to their degrees, we determine the forgotten topological index of line graphs of certain molecular graphs of drug structures. The result achieved in this paper illustrates the promising prospects of the applications for pharmacological engineering.

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