e-ISSN: 2582-5208
International Research Journal of Modernization in Engineering Technology and Science
(Peer-Reviewed, Open Access, Fully Refereed International Journal)
Volume:03/Issue:06/June-2021 Impact Factor- 7.868 www.irjmets.com

FORGOTTEN TOPOLOGICAL INDEX OF SUBDIVISION GRAPH AND LINE GRAPH OF GRAPHENE

Ashwini Yalnaik*1, Hemaraddi Maraddi*2

*1Department of Studies in Mathematics, Davanagere University, Davanagere – 577007, India.

*2Department of Mathematics, karnatak science College, Dharwad-580001, India.

DOI : https://www.doi.org/10.56726/IRJMETS13935

ABSTRACT

The forgotten topological index widely used in the analysis of drug molecular structures, which is helpful for pharmaceutical and medical scientists to grasp the biological and chemical characteristics of new drugs. In this paper we present the Forgotten index of subdivision graph and line graph of widely used chemical structure graphene.

Keywords: Forgotten topological index, line graph, subdivision graph

Mathematics Subject Classification: 05C07,92E10

I. INTRODUCTION

Development of drugs in medicine industry has more demand to determine the pharmaco- logical, chemical and biological characteristic of these new drugs.In theoretical chemistry, chemical compounds and drugs are modeled as graphs in which each vertex represents an atom of molecule and covalent bounds between atoms are represented by edges between the corresponding vertices. Such a graph constructed according to a chemical compoundsis often called its molecular graph. May previous studies have pointed out that chemicaland pharmacodynamics characteristics of drugs and their molecular structures are closely correlated [2, 5, 6, 7, 9, 10]. In mathematical chemistry, numbers encoding certain structural features of organic moleculesand derived from the corresponding molecular graph, are called graph invariants or more commonly topological indices. In mathematical medicine the structure of the drug is represented as an undirected graph. Where each vertex indicates an atom and each edge

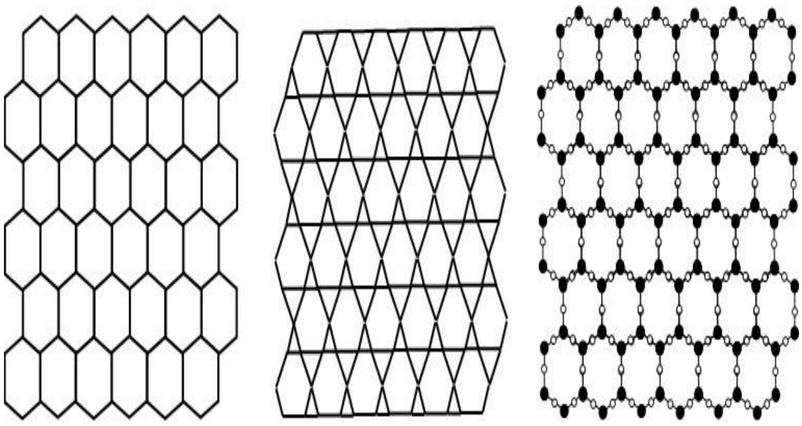

Figure 1: 2-Dimensional graph of graphene sheet and its line graph and subdivisiongraph

represents a chemical bond between the atoms.

Let G be a simple graph corresponding to a drug structure with vertex(atom) set V (G) and edge(bond) set E(G). The edge between adjacent vertices u and v is denoted by uv. Thus if uv ∈ E(G) then u and v are adjacent in G. The degree of a vertex u denoted by $d_G(u) = d(u)$ is the number of edges incident to u. The subdivision graph S(G) is thegraph obtained from G by replacing each of its edge by a path of length 2, or equiva- lently, by inserting an additional vertex into each edge of G. The line graph of a graphG, denoted by L(G) is the graph whose vertices has one to one correspondence with the edges of G and two vertices in L(G) are adjacent if and only if the corresponding edges are adjacent in G.For a graph theoretic terminology, we refer the books [1, 8]. In this paper we carried out the further studies of the paper[4] and obtained forgotten index ofsubdivision graph and line graph of graphene.

1. Line graph and subdivision graph of graphene

Theorem 2.1. Let G(m,n) be a graphene sheet with n-rows and m-columns as in Fig.1, then

$$F[L(G(m,n))] = \begin{cases} 192mn - 2n - 20m - 140 & \text{if } n \neq 1 \\ 172m - 124 & \text{if } n = 1 \end{cases}$$

Proof. If if $n \neq 1$then by analysis of structure of line graph of graphene sheet G(m,n)we partition the vertex set of $L[G(m,n)]$ into three subsets as $V_1 = \{u/d(u) = 2\}$,$V_2 = \{u/d(u) = 3\}$ and $V_3 = \{u/d(u) = 4\}$. Let d_i denotes number of vertices whose the degree of vertex is i. The number of vertices on each row of line graph of graphane sheet$G(m,n)$ is given in the Table 1. Using the data of Table 1, we can easily write that

$|V_1| = n + 4$, $|V_2| = 2n + 4m - 4$, $|V_3| = 3mn - n - 2m - 1$

Therefore, using the definition of forgotten topological index, we obtain

Table 1: Number of vertices in each row of $L[G(m,n)]$.

Row	d_2	d_3	d_4
1	3	2(m-1)+2	3(m-1)+1
2	1	2	3m-1
3	1	2	3m-1
.	.	.	.
.	.	.	.
.	.	.	.
.	.	.	.
.	.	.	.
n-1	1	2	3m-1
n	3	2(m-1)+2	m-1

$$F[L(G(m,n))] = \sum_{u \in V(L[G(m,n)])} (d(u))^3$$

$$= \sum_{u \in V_1} (d(u))^3 + \sum_{u \in V_2} (d(u))^3 + \sum_{u \in V_3} (d(u))^3$$

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

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

If $n = 1$ then by the direct observation, $|V_1| = 6$, $|V_2| = 4(m-1)$, $|V_3| = n - 1$, theforgotten index of $L[G(m,n)]$ when n=1 is

$F[L(G(m,n))] = 172m - 124$.

Theorem 2.2. Let G(m,n) be a graphene sheet with n-rows and m-columns as in Fig.1, then we obtain

$$F[S(G(m,n))] = \begin{cases} 78mn + 32m + 32n - 46 & \text{if } n \neq 1 \\ 110m - 14 & \text{if } n = 1 \end{cases}$$

Proof. If $n = 1$ and $m \geq 1$, then we get the result by putting $n = 1$ in case (i). Now for $n \geq 2$ and $m \geq 1$, by analysis of structure of line graph of graphene sheet $G(m,n)$,we partition the vertex set of S[G(m, n)] into two subsets as $V_1 = \{u/d(u) = 2\}$ and$V_2 = \{u/d(u) = 3\}$. The number of vertices on each row of line graph of graphane sheet $S[G(m,n)]$ is given in the Table 1. Using the data of Table 2, we can easily write that

$|V_1| = 3mn + 4m + 4n + 1$ and $|V_2| = 2mn - 2$

Table 2: Number of vertices in each row of $G(m,n)$.

Row	d_2	d_3
1	6m+4	3m-1

2	3m+4	2m
3	3m+4	2m
.	.	.
.	.	.
.	.	.
	.	.
n-1	3m+4	2m
n	4m+5	m-1

Therefore, using the definition of forgotten topological index, we obtain

$$F[S(G(m,n))] = \sum_{u\in V(L[G(m,n))])} (d(u))^3$$

$$= \sum_{u\in V_1} (d(u))^3 + \sum_{u\in V_2} (d(u))^3$$

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

$$= 78mn + 32m + 32n - 46 .$$

If $n = 1$ then by the direct observation, we have

$F[L(G(m,n))] = 110m - 14.$

II. CONCLUSION

In this work, we obtain forgotten topological index of subdivision graph and line graph of graphene structure which is widely used in pharmaceutical field. Further, one can obtain the other topological index of this structure and can establish the other properties of graphene structure with usage of topological indices.

III. REFERENCES

[1] F. Buckley, F. Harary, Distance in Graphs, Addison-Wesley, Redwood, California,1990.

[2] M.R. Farahani, M.K. Jamil and M. Imran, (2016), Vertex PIn Topological Index of Titania Carbon Nanotubes TiO2(m;n), Applied Mathematics and Nonlinear Sci- ences, 1, No 1, 175-182. doi 10.21042/AMNS.2016.1.00013

[3] B. Furtula, I. Gutman, A forgotten topological index, J. Math. Chem. 53 (4) (2015),1184–1190.

[4] Wei Gao, Muhammad Kamran Siddiqui, Muhammad Imran, Muhammad Kamran Jamil, Mohammad Reza Farahani, Forgotten topological index of chemical structure in drugs, Saudi Pharmaceutical Journal 24 (2016), 258–264.

[5] W. Gao, M. R. Farahani, Computing the reverse eccentric connectivity index for certain family of nanoconec and fullerene structures, J. Nanotechnol 2016, 6 (2016), http://dx.doi.org/10.1155/2016/3129561. Article ID 3129561.

[6] W. Gao, M. R. Farahani, Degree-based indices computation for special chemical molecular structures using edge dividing method, Appl. Math. Nonlinear Sci., 1(1) (2016), 94–117.

[7] W. Gao, M. R. Farahani, L. Shi, The forgotten topological index of some drugstructures, Acta Medica, Mediteranea,32 (2016), 579–585.

[8] F. Harary, Graph Theory, Narosa Publishing House, New Delhi,1999.

[9] H. S. Ramane and R. B. Jummannaver, Note on forgotten topological index ofchemical structure in drugs, Applied Mathematics and Nonlinear Sciences 1(2) (2016) 369–374

[10] L. Yan, W. Gao, J.S. Li, General harmonic index and general sum connectivity index of polyomino chains and nanotubes, J. Comput. Theor. Nanosci, 12(10) (2015), 3940– 3944.