JAMI
Journal of Applied Mathematics and Informatics
J. Appl. Math. & Informatics Vol. **42***(2024), No. 1, pp. 159 - 167*
https://doi.org/10.14317/jami.2024.159

STUDY ON LINE GRAPH OF SOME GRAPH OPERATORS OF CHEMICAL STRUCTURES VIA F AND M_1 INDICES

P.S. HEMAVATHI*, M. MANJUNATH, M. PRALAHAD AND S.M. VEERESH

Abstract. The Topological indices are known as Mathematical characterization of molecules. In this paper, we have studied line graph of subdivision and semi-total point graph of triangular benzenoid, polynomino chains of 8-cycles and graphene sheet through forgotten and first Zagreb indices.

AMS Mathematics Subject Classification: 05C09, 05C92.
Key words and phrases : Line graph, subdivision graph, semi-total point graph, F-index, M_1-index, triangular benzenoid, polynomino chains, graphene sheet.

1. Introduction

A topological index is a numerical parameter which characterizes its molecular topology and used for quantitative structure activity relationship ($QSAR$) and quatitative structure property relationship ($QSPR$). In 1947, the first topological index (named as Wiener index or path index) was introduced by Wiener for finding the boiling point of paraffins [5]. For new topological indices, we suggest the reader to refer the papers [7, 9–20].

In [1] , B. Furtula and et al., proposed a topological index based on the degrees of vertices of graph, which is known as forgotten index and it is defined as

$$F[G] = \sum_{u \in V[G]} deg_G^3 u$$

or

Received June 22, 2023. Revised October 6, 2023. Accepted October 18, 2023. *Corresponding author.

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

The first Zagreb index is introduced by Gutman et al. [2] and it is defined as

$$M_1(G) = \sum_{uv \in E(G)} [deg_G(u) + deg_G(v)]$$

or

$$M_1(G) = \sum_{u \in V(G)} deg_G^2(u)$$

Definition 1.1. [6] The **line graph** $L(G)$ is the graph obtained by associating a vertex with each edge of the graph G and two vertices are adjacent with an edge iff the corresponding edges of G are adjacent.

Definition 1.2. [21] The **subdivision graph** $S(G)$ is the graph obtained by replacing each of its edge by a path of length 2 or equivalently, by inserting an additional vertex into each edge of G.

Definition 1.3. The **semi-total point graph** $R(G)$ graph is obtained from G by adding a new vertex corresponding to every edge of G and by joining each new vertex to the end vertices of the edge corresponding to it.

Triangular benzenoid: Benzenoid molecular graph is a connected geometric figure obtained by arranging congruent regular hexagons in a plane so that two hexagons are either disjoint or have a common edge and it is shown in below Figure 1 [3, 18, 22].

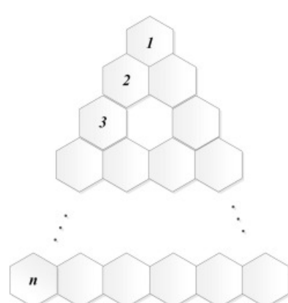

FIGURE 1. Triangular benzenoid

Polynomino chains of 8-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 $4k$-cycle of length one and Polynomino chains of 8-cycles shown in below Figure 2.

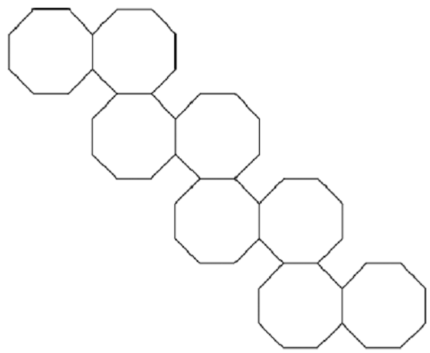

FIGURE 2. Polynomino chains of 8-cycles

Graphene sheet: Graphene sheets are essentially the finest materials in the world. Graphene sheet is a one-atom-thick planar sheet of carbon iotas which are intensively packed in a hexagonal lattice structure. Graphene sheets show high electrical conductance at room temperatures and molecular graph of graphene sheet as shown in below Figure 3 (See [4, 8]).

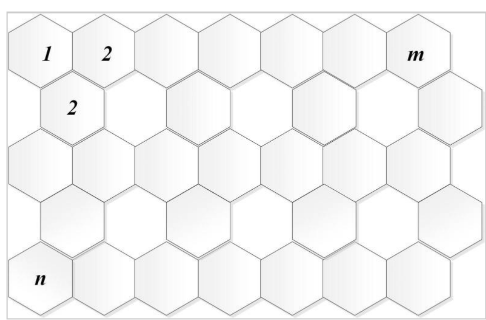

FIGURE 3. Graphene sheet

2. Main results

In this section, we compute the forgotten and first Zagreb indices of line graph of subdivision and semi-total point graph of triangular benzenoid, polynomino chains of 8-cycles and graphene sheet.

Theorem 2.1. *Let Γ be the line graph of subdivision graph of triangular benzenoid, then*

$$\begin{aligned} M_1[\Gamma] &= \frac{9}{2}(n^2-n+8)^2+\frac{27}{4}(n^2+7n-8)^2, \\ F[\Gamma] &= \frac{27}{4}(n^2-n+8)^3+\frac{81}{8}(n^2+7n-8)^3. \end{aligned}$$

Proof. Let Γ be a line graph of subdivision graph of triangular benzenoid. Applying the line and subdivision operations to Figure 1, we obtain the two types of vertices based on their degrees and which are shown in the below **Table 1**.

Table 1. Degree partition of Γ based on their degrees.

$deg_\Gamma(u)$	Number of vertices
2	$12+\frac{3n(n-1)}{2}$
3	$\frac{3}{2}(n^2+7n-8)$

Consider,

$$\begin{aligned} M_1[G] &= \Sigma_{u\in V[G]} deg_G^2 u \\ M_1[\Gamma] &= 2\left(12+\frac{3n(n-1)}{2}\right)^2+3\left(\frac{3}{2}(n^2+7n-8)\right)^2 \\ &= \frac{1}{2}(24+(3n(n-1)))^2+\frac{3^3}{2^2}(n^2+7n-8)^2 \\ M_1[\Gamma] &= \frac{9}{2}(n^2-n+8)^2+\frac{27}{4}(n^2+7n-8)^2. \end{aligned}$$

the above proof method is also follows for $F[\Gamma]$. □

Theorem 2.2. *Let Υ be the line graph of semi-total point graph of triangular benzenoid, then*

$$\begin{aligned} M_1[\Upsilon] &= 9(n^2-n+8)^2+\frac{27}{2}(n^2+7n-4)^2+18n^2(n-1)^2+360(n-1)^2, \\ F[\Upsilon] &= \frac{27}{2}(n^2-n+8)^3+\frac{81}{4}(n^2+7n-8)^3+27(n(n-1))^3+2160(n-1)^3. \end{aligned}$$

Proof. Let Υ be a line graph of semi-total point graph of triangular benzenoid. Applying the line and semi-total point operations to Figure 1, we obtain the four types of vertices based on their degrees and which are shown in the below **Table 2**.

Table 2. Degree partition of Υ based on their degrees.

$deg_\Upsilon(u)$	Number of vertices
4	$12+\frac{3n(n-1)}{2}$
6	$\frac{3}{2}(n^2+7n-8)+6$
8	$\frac{3n(n-1)}{2}$
10	$6(n-1)$

Consider,

$$\begin{aligned} M_1[G] &= \Sigma_{u\in V[G]} deg_G^2 u \\ M_1[\Upsilon] &= 4\left(12+\frac{3n(n-1)}{2}\right)^2+6\left(\frac{3}{2}(n^2+7n-8)+6\right)^2 \\ &+ 8\left(\frac{3n(n-1)}{2}\right)^2+10(6(n-1))^2 \\ M_1[\Upsilon] &= 9(n^2-n+8)^2+\frac{27}{2}(n^2+7n-4)^2+18n^2(n-1)^2+360(n-1)^2. \end{aligned}$$

the above proof method is also follows for $F[\Upsilon]$. □

Theorem 2.3. *Let Φ be the line graph of subdivision graph of polynomino chains of 8-cycles, then*

$$\begin{aligned} M_1[\Phi] &= 3776n^2-160n+236, \\ F[\Phi] &= 107008n^3-3618n^2+20064n+376. \end{aligned}$$

Proof. Let Φ be a line graph of subdivision graph of polynomino chains of 8-cycles. Applying the line and subdivision operations to Figure 2, we obtain the two types of vertices based on their degrees and which are shown in the below **Table 3**.

Table 3. Degree partition of Φ based on their degrees.

$deg_\Phi(u)$	Number of vertices
2	$32n+8$
3	$24n-6$

Consider,

$$\begin{aligned} M_1[G] &= \Sigma_{u\in V[G]} deg_G^2 u \\ M_1[\Phi] &= 2(32n+8)^2+3(24n-6)^2 \\ M_1[\Phi] &= 3776n^2-160n+236. \end{aligned}$$

the above proof method is also follows for $F[\Phi]$. □

Theorem 2.4. *Let Ψ be the line graph of semi-total point graph of polynomino chains of 8-cycles, then*

$$\begin{aligned} M_1[\Psi] &= 13024n^2-320n+178, \\ F[\Psi] &= 420224n^3-49920n^2+18672n-62. \end{aligned}$$

Proof. Let Ψ be a line graph of semi-total point graph of polynomino chains of 8-cycles. Applying the line and semi-total point operations to Figure 2, we obtain the four types of vertices based on their degrees and which are shown in the below **Table 4**.

Table 4. Degree partition of Ψ based on their degrees.

$deg_{\Psi}(u)$	Number of vertices
4	$32n + 4$
6	$36n - 2$
8	$8n$
10	$8n - 3$

Consider,

$$\begin{aligned} M_1[G] &= \Sigma_{u \in V[G]} deg_G^2 u \\ M_1[\Psi] &= 4(32n+4)^2 + 6(36n-2)^2 + 8(8n)^2 + 10(8n-3)^2 \\ M_1[\Psi] &= 13024n^2 - 320n + 178. \end{aligned}$$

the above proof method is also follows for $F[\Psi]$. □

Theorem 2.5. *Let $\gimel$ be the line graph of subdivision graph of graphene sheet with n-rows and m-columns, then*

$$\begin{aligned} M_1[\gimel] &= 32(m+n+1)^2 + 12(|E(\gimel(m,n))| - 2m - 2n - 2)^2, \\ F[\gimel] &= 128(m+n+1)^3 + 24(|E(\gimel(m,n))| - 2m - 2n - 2)^3. \end{aligned}$$

Proof. Let $\gimel$ be a line graph of subdivision graph of graphene sheet with n-rows and m-columns. Applying the line and subdivision operations to Figure 3, we obtain the two types of vertices based on their degrees and which are shown in the below **Table 5**.

Table 5. Degree partition of $\gimel$ based on their degrees.

$deg_{\gimel}(u)$	Number of vertices
2	$4m + 4n + 4$
3	$2\vert E(\gimel(m,n))\vert - 4m - 4n - 4$

Consider,

$$\begin{aligned} M_1[G] &= \Sigma_{u \in V[G]} deg_G^2 u \\ M_1[\gimel] &= 2(4m+4n+4)^2 + 3(2|E(\gimel(m,n))| - 4m - 4n - 4)^2 \\ M_1[\gimel] &= 32(m+n+1)^2 + 12(|E(\gimel(m,n))| - 2m - 2n - 2)^2. \end{aligned}$$

the above proof method is also follows for $F[\gimel]$. □

Theorem 2.6. *Let $\daleth$ be the line graph of semi-total point graph of polynomino chains of 8-cycles, then*

$$\begin{aligned} M_1[\daleth] &= 64(m+n+1)^2 + 6(2|E(\daleth(m,n))| - 4m - 3n)^2 \\ &+ 32(2m+n-2)^2 + 10(|E(\daleth(m,n))| - 4m - 3n)^2, \\ F[\daleth] &= 256(m+n+1)^3 + 6(2|E(\daleth(m,n))| - 4m - 3n)^3 \end{aligned}$$

$$+ \quad 64(2m+n-2)^3 + 10(|E(\urcorner(m,n))| - 4m - 3n)^3.$$

Proof. Let $\urcorner$ be a line graph of semi-total point graph of graphene sheet with n-rows and m-columns. Applying the line and semi-total point operations to Figure 3, we obtain the four types of vertices based on their degrees and which are shown in the below **Table 6**.

Table 6. Degree partition of $\urcorner$ based on their degrees.

$deg_{\neg}(u)$	Number of vertices
4	$4m+4n+4$
6	$2\lvert E(\urcorner(m,n))\rvert - 4m - 3n$
8	$4m+2n-4$
10	$\lvert E(\urcorner(m,n))\rvert - 4m - 3n$

Consider,

$$\begin{aligned}
M_1[G] &= \Sigma_{u \in V[G]} deg_G^2 u \\
M_1[\urcorner] &= 4(4m+4n+4)^2 + 6(2|E(\urcorner(m,n))| - 4m - 3n)^2 \\
&+ 8(4m+2n-4)^2 + 10(|E(\urcorner(m,n))| - 4m - 3n)^2 \\
M_1[\urcorner] &= 64(m+n+1)^2 + 6(2|E(\urcorner(m,n))| - 4m - 3n)^2 \\
&+ 32(2m+n-2)^2 + 10(|E(\urcorner(m,n))| - 4m - 3n)^2.
\end{aligned}$$

the above proof method is also follows for $F[\urcorner]$. □

3. Conclusion

In this article, we have calculated the forgotten and first Zagreb indices of line graph of subdivision and semi-total point graph of triangular benzenoid, polynomino chains and graphene sheet. These results are useful to study the $QSPR$ and $QSAR$ of above chemical molecules.

Conflicts of interest : The authors declare no conflict of interest.

Data availability : Not applicable

Acknowledgments : The authors would like to thank the referees for their invaluable comments and suggestions which led to the improvement of the manuscript.

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P.S. Hemavathi received doctorate from VSK University in 2019. She has published 15 research articles in internationally reputed journals. She presented research articles in 10 reputed conferences. She is working as Assistant Professor in the Department of Mathematics, Siddagangai Institute of Technology, Tumakur, India.

Department of Mathematics, Siddaganga Institute of Technology, Tumakur, Karnataka, India.
e-mail: hemavathisuresh@gmail.com

Manjunath Muddalapuram graduated and received his M.Sc. degree from Gulbarga University. He also received doctorate from VSK University in 2020. He has published 25 research articles in internationally reputed journals. He presented research articles in 15 reputed conferences. He is actively visiting IITs and reputed Institutions for workshop and short visits for research work. He joined as Assistant Professor in the Department of Mathematics, Ballari Institute of Technology and Management, Ballari in the year 2020.

Department of Mathematics, Ballari Institute of Technology and Management, Ballari, Karnataka, India.
e-mail: manju3479@gmail.com

Pralahad Mahagaonkar graduated and received his M.Sc. degree from Gulbarga University. He also received his doctorate from Gulbarga University in 2011. He has published 10 research articles in internationally reputed journals. He presented research articles in 15 reputed conferences. He is actively visiting reputed Institutions for workshop and short visits for research work. He working as Associate Professor in the Department of Mathematics, Ballari Institute of Technology and Management, Ballari.

Department of Mathematics, Ballari Institute of Technology and Management, Ballari, Karnataka, India.
e-mail: pralahadm74@gmail.com

S.M. Veeresh graduated and received his M.Sc. degree from Gulbarga University. He started his doctoral programme in 2016 at R and D center, Department of Mathematics, Ballari Institute of Technology and Management, Ballari, Karnataka under Visvesvaraya Technological University, Belagavi, Karnataka. He has published 4 research articles in internationally reputed journals. He presented research articles in 6 reputed conferences. He is actively visiting reputed Institutions for workshop and short visits for research work. He joined as Assistant Professor in the Department of Mathematics, Ballari Institute of Technology and Management, Ballari in the year 2013.

Department of Mathematics, Ballari Institute of Technology and Management, Ballari, Karnataka, India.
e-mail: veeresh2010.1155@gmail.com