UMT PRESS

Journal of Mathematical Sciences and Informatics
Journal Homepage: https://journal.umt.edu.my/index.php/jmsi
eISSN: 2948-3697
DOI: http://doi.org/10.46754/jmsi.2025.12.003

TOPOLOGICAL INDICES OF LINE AND PARALINE GRAPHS OF CONDUCTIVE 2D METAL-ORGANIC FRAMEWORKS (MOFs)

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ARTICLE INFO

Article History:
Received 22 July 2025
Revised 3 October 2025
Accepted 3 October 2025
Published 15 December 2025

Keywords:
Topological indices;
line graph;
paraline graph.

ABSTRACT

Topological indices assign a numerical value to a chemical structure. The use of these graph indices in chemical graph theory is very broad. In this article, we calculate several well-known degree-based topological indices for the chemical structures of conductive 2D Metal-organic Frameworks (MOFs) by applying the concept of line and paraline graphs. These results are instrumental in the design of emerging networks, enabling the study of their topological indices to gain a deeper understanding of their underlying topology.

2020 Mathematics Subject Classification: 05C10, 05C12, 05C90

Introduction

A molecular topographical depiction is a representation of the structural formula of a chemical combination in a restricted sketch explanation, whose vertices conform to the atoms of the combination and edges conform to chemical bonds. The concept of topological index originated from work done by Wiener [1] while he was studying the boiling point of paraffin. He named this index as the path number. Later, the path number was renamed as the Wiener index. The Wiener index is the first and most studied topological index, both from a theoretical point of view and in applications, and it is defined as the sum of distances between all pairs of vertices in G [2, 3]. The theory of topological indices is a very extensive area of research in chemistry and chemical graph theory.

A graph G with vertex set $V(G)$ and edge set $E(G)$ is connected if there exists a relationship between any pair of vertices in G. A network is simply a connected graph, having no multiple edges and no loops. For a graph G, the degree of a vertex v is the number of edges incident on v and is denoted by d_v. Given a graph G, the line graph $L(G)$ is a graph such that each vertex of $L(G)$ represents an edge of G and two vertices in $L(G)$ are adjacent if and only if their corresponding edges in G share a common vertex. A paraline graph is the graph obtained by subdividing its line graph. The fact that many interesting graphs are composed of simpler graphs that serve as their basic building blocks. Many chemists and mathematicians have been studying the properties of line graphs and subdivision graphs.

Various mathematical representations, such as numbers, polynomials, sequences, or matrices, can uniquely identify graphs. A topological index is a specific type of numerical descriptor that captures a graph's topology and remains unchanged even if the graph is rearranged. Topological indices are broadly categorised into distance-based topological indices, degree-based topological indices, and counting-related polynomials and indices. Among these, degree-based topological indices are particularly significant in chemical graph theory and play a crucial role in the field of chemistry.

The Randić connectivity index, introduced by Randić [4] in 1975, has a generalised form known as the general Randić connectivity index or general product-connectivity index. It is calculated using the following formula:

$$R_\alpha = \sum_{uv \in E(G)} (d_u d_v)^\alpha. \tag{1}$$

Here, α is a real number, and the sum is taken over all edges (u, v) in the graph G, where d_u and d_v are the degrees of vertices u and v, respectively.

Later, Zhou and Trinajstić [5, 6] proposed the related concepts of the sum-connectivity index and the general sum-connectivity index for a graph. The general sum-connectivity index is defined as:

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha , \tag{2}$$

where α is a real number. The first general Zagreb index was studied in Li and Zhao [7]:

$$M_\alpha(G) = \sum_{u \in V(G)} (d_u)^\alpha, \tag{3}$$

with α a real number. Estrada *et al*. [8] introduced the atom-bond connectivity (ABC) index:

$$ABC(G) = \sum_{uv \in V(G)} \sqrt{\frac{d_u + d_v - 2}{d_u x\, d_v}}, \tag{4}$$

The concept of geometric-arithmetic (GA) index was introduced in Vukičević and Furtula [9] and is defined as:

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u x\, d_v}}{d_u + d_v}, \tag{5}$$

In 2010, Ghorbani and Hosseinzadeh [10] introduced the fourth variation of the ABC index, defined as:

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u\, x\, S_v}}, \tag{6}$$

here, S_u represents the sum of the degrees of all vertices adjacent to vertex u. More recently, in 2011, Graovac *et al*. [11] proposed the fifth version of the GA index, which is defined as:

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u\, x\, S_v}}{S_u + S_v}, \tag{7}$$

Shirdel *et al*. [12] introduced a new degree-based Zagreb index named "hyper-Zagreb index" as:

$$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2. \tag{8}$$

Ghorbani and Azimi [13] defined two new versions of Zagreb indices of a graph G. The first multiple Zagreb index $PM_1(G)$, second multiple Zagreb index $PM_2(G)$, first Zagreb polynomial $M_1(G, x)$, and second Zagreb polynomial $M_2(G, x)$ are defined as:

$$PM_1(G) = \prod_{uv \in E(G)} d_u + d_v, \tag{9}$$

$$PM_2(G) = \prod_{uv \in E(G)} d_u \; x \; d_v, \tag{10}$$

$$M_1(G, x) = \sum_{uv \in E(G)} x^{(d_u + d_v)}, \tag{11}$$

$$M_2(G, x) = \sum_{uv \in E(G)} x^{(d_u \, x \, d_v)}. \tag{12}$$

Nowadays, there is extensive research activity on ABC and GA indices and their variants, as can be additionally observed [10, 14]. The topological indices ABC_4 and GA_5 for silicate, chain silicate, oxide, honeycomb, and hexagonal networks are discussed in Hayat and Imran [15]. Imran *et al*. [16] computed ABC and GA indices for the oxide and chain silicate networks and additionally for butterfly and Benes networks. For further study of the topological indices of some graph families, please refer to Ahmad *et al*. [17, 18], Baca *et al*. [19], Baig *et al*. [20], Elahi *et al*. [21, 22], Hayat and Imran *et al*. [23, 24], and Nadeem *et al*. [14].

In this article, we study several well-known degree-based topological indices for the chemical structures of conductive 2D MOFs, motivated by the results in Ahmad *et al*. [17] and Nadeem *et al*. [14, 25], and by applying the concept of line and paraline graphs.

Results and Discussions

In recent years, there has been increasing interest in utilising metal-organic frameworks (MOFs) as next-generation functional materials in electronic and optoelectronic devices. Metal-organic frameworks (MOFs) are highly sought after for sensor applications due to their large surface area and customisable chemical properties, achieved through a "bottom-up" synthetic method. However, their use in electronic devices has been limited because most MOFs lack high electrical conductivity. A recent development in this area is Cu_3 (HITP = 2,3,6,7,10,11-hexaiminotriphenylene), a newly created 2D MOF that exhibits electrical conductivity.

Graph theory is increasingly important because it enables the creation of models across diverse fields like computer science, mathematics, genetics, chemistry, telecommunications, and engineering. Specifically, in chemistry, graph theory offers a way to develop computer algorithms that can identify various connections and behaviours within chemical structures.

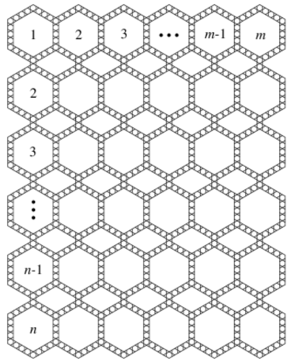

Figure 1: Graph G_L of the line graph of chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$

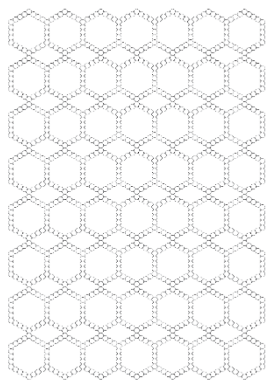

Figure 2: Graph G_{LP} of the line graph of chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$

Let G_L and G_{LP} be the graphs of the line and paraline graphs of the chemical structures of the conductive 2D MOFs as shown in Figures 1 and 2. A paraline graph is also known as the line graph of the subdivision graph of the original graph. These graphs consist of main hexagons and minor hexagons. To avoid confusion, we use the term paraline graph instead of the line graph of the subdivision graph. The methodological steps are as follows: Construction of GL and GLP, identification of vertex degrees, application of the formula, and derivation of general results. For simplicity, imagine a structure with m main hexagons in each row and n main hexagons in each column. This structure, represented as G_L, contains a total of $2m + 4n$ vertices. Among these, $60mn + 20n + 4m$ vertices have a degree of 2, and $33mn + 2n - 5m$ vertices have a degree of 3. The number of vertices in G_{LP} is $186mn + 52n + 2m$, among which $60mn + 28n + 8m$ vertices are of degree 2 and $126mn + 24n - 6m$ vertices are of degree 3.

Let $\delta(G_L)$ and $\Delta(G_L)$ be the minimum and maximum degrees of G_l, respectively. The edge set $E(G_l)$ can be divided into several partitions: For any i and j,$\delta(G_l) \leq i, j \leq \Delta(G_l)$, let

$$E_{ij} = \{ e = uv \in E(G_l) : d(v) = i, d(u) = j \}, e_{ij} = |E_{ij}|,$$

and

$$V_i = \{ v \in V(G_L) : d(v) = i \}, n_i = |V_i|.$$

Let $\delta(G_{LP})$ and $\Delta(G_{LP})$ be the minimum and maximum degrees of G_{LP}, respectively. The edge set $E(G_{LP})$ can also be divided into several partitions: For any i and j, $\delta(G_{LP}) \leq i, j \leq \Delta(G_{LP})$, let

$$E_{ij} = \{ e = uv \in E(G_l) : d(v) = i, d(u) = j \}, e_{ij} = |E_{ij}|,$$

and

$$V_i = \{ v \in V(G_L) : d(v) = i \}, n_i = |V_i|.$$

Table 1: Edge partition of the graph G_L

(d_u, d_v) where $uv \in E(G_L)$	(2,3)	(3,3)	(3,3)	(4,4)
Number of edges	$8n + 4m$	$50mn + 18n + 4m$	$80mn + 16n$	$26mn - 4n - 10m$

Table 2: Edge partition of the graph G_{PL}

(d_u, d_v) where $uv \in E(G_{PL})$	(2,2)	(2,3)	(3,3)
Number of edges	$30mn + 18n + 6m$	$60mn + 20n + 4m$	$159mn + 26n - 11m$

Theorem 1. Let's define G_L and G_{LP} graphs, where m represents the number of main hexagons in each row and n represents the number of main hexagons in each column. Then:

$$M_\alpha(G_L) = (2m + 4n)2^\alpha + (60mn + 4m + 20n)3^\alpha + (33mn - 5m + 2n)4^\alpha,$$

$$M_\alpha(G_{LP}) = (60mn + 28n + 8m)2^\alpha + (126mn + 24n - 6m)3^\alpha,$$

$$R_\alpha(G_L) = (4m + 8n)6^\alpha + (50mn + 18n + 4m)9^\alpha + (80mn + 16n)12^\alpha + (26mn - 10m - 4n) \cdot 16^\alpha,$$

$$R_\alpha(G_{LP}) = (4m + 8n)6^\alpha + (50mn + 18n + 4m)9^\alpha + (80mn + 16n)12^\alpha + (26mn - 10m - 4n)16^\alpha,$$

$$\chi_\alpha(G_L) = (4m + 8n)5^\alpha + (50mn + 18n + 4m)6^\alpha + (80mn + 16n)7^\alpha + (26mn - 10m - 4n)8^\alpha,$$

$$\chi_\alpha(G_{LP}) = (30mn + 18n + 6m)4^\alpha + (60mn + 20n + 4m)5^\alpha + (159mn + 26n - 11m)6^\alpha,$$

where α is a real number.

Proof. The graphs G_L and G_{LP} are shown in Figures 1 and 2, respectively. The total number of edges in G_L is $(156mn + 38n - 2m)$ and the total number of edges in G_{LP} is $(249mn + 64n - m)$. For the edge partition of graphs G_L and G_{LP}, the degree of the end vertices of each edge is shown in Tables 1 and 2. We apply Formulas 1, 2, and 3 to the information in Tables 1 and 2, obtaining the required results.

Theorem 2. Let G_L and G_{LP} be the line graph and paraline graph of chemical structures of the conductive 2D MOFs. Then:

$$GA(G_L) = \frac{2}{5}(4m + 8n)\sqrt{6} + 76mn + 14n - 6m + \frac{4}{7}(80mn + 16n)\sqrt{3},$$

$$GA(G_{LP}) = 189mn + 44n - 5m + \frac{2}{5}(60mn + 20n + 4m)\sqrt{6}.$$

Proof. The edge partition of graphs G_L and G_{LP} based on the degree of the end vertices of each edge is shown in Tables 1 and 2. We apply Formula 5 to the information in Tables 1 and 2, obtaining the required results. This completes the proof.

Theorem 3. Let G_L and G_{LP} be the line graph and paraline graph of chemical structures of the conductive 2D MOFs. Then:

$$\begin{aligned} ABC_4(G_L) = {} & \frac{1}{18}(4m + 8n)\sqrt{78} + \left(\frac{1}{30}\right)(4m + 8n)\sqrt{170} + \left(\frac{2}{39}\right)(4m + 8n)\sqrt{65} \\ & + \left(\frac{3}{10}\right)(30mn + 4m + 14n)\sqrt{2} + \left(\frac{1}{110}\right)(20mn - 4m - 4n)\sqrt{2090} \\ & + \left(\frac{1}{6}\right)(40mn + 8n)\sqrt{6} + \left(\frac{1}{130}\right)(4m + 8n)\sqrt{2730} + \left(\frac{1}{13}\right)(4m + 8n)\sqrt{26} \\ & + \left(\frac{1}{154}\right)(36mn - 8m - 16n)\sqrt{3542} + \left(\frac{2}{55}\right)(4mn + 4m)\sqrt{110} \\ & + \left(\frac{5}{182}\right)(4m + 8n)\sqrt{182} + \left(\frac{1}{14}\right)(16mn - 4m - 12n)\sqrt{26} \\ & + \left(\frac{3}{70}\right)(4mn - 4m)\sqrt{70} + \left(\frac{2}{15}\right)(2mn - 2m)\sqrt{7} + \left(\frac{1}{60}\right)(4mn - 4m)\sqrt{435}, \end{aligned}$$

$$\begin{aligned} ABC_4(G_{LP}) = {} & \left(\frac{1}{4}\right)(4n + 2m)\sqrt{6} + \left(\frac{1}{10}\right)(8n + 4m)\sqrt{35} + \left(\frac{2}{5}\right)(30mn + 6n)\sqrt{2} + \\ & \left(\frac{1}{20}\right)(60mn + 20n + 4m)\sqrt{110} + \left(\frac{1}{8}\right)(20mn + 12n + 4m)\sqrt{14} + \\ & \left(\frac{1}{12}\right)(80mn + 16n)\sqrt{30} + \left(\frac{236}{9}\right)mn - \left(\frac{8}{9}\right)n - \left(\frac{20}{3}\right)m. \end{aligned}$$

Proof. Let G_L and G_{LP} be the line graph and paraline graph of chemical structures of the conductive 2D MOFs. There are *4m + 8n* edges between vertices of sum of degree 6 and sum of degree 9, *4m + 8n* edges between vertices of sum of degree 9 and sum of degree 10, *4m + 8n* edges between vertices of sum of degree 9 and sum of degree 13, *30mn + 4m + 14n* edges between vertices of sum of degree 10 and sum of degree 10, *20mn – 4m – 4n* edges between vertices of sum of degree 10 and sum of degree 11, *40mn + 8n* edges between vertices of sum of degree 10 and sum of degree 12, *4m + 8n* edges between vertices of sum of degree 10 and sum of degree 13, *4m + 8n* edges between vertices of sum of degree 11 and sum of degree 13, *36mn – 8m – 16n* edges between vertices of sum of degree 11 and sum of degree 14, *4mn + 4m* edges between vertices of sum of degree 11 and sum of degree 15, *4m + 8n* edges between vertices of sum of degree 13 and sum of degree 14, *16mn – 4m*

– *12n* edges between vertices of sum of degree 14 and sum of degree 14, *4mn – 4m* edges between vertices of sum of degree 14 and sum of degree 15, *2mn – 2m* edges between vertices of sum of degree 15 and sum of degree 15, and *4mn – 4m* edges between vertices of sum of degree 15 and sum of degree 16 for the graph G_L.

There are *4n + 2m* edges between vertices of sum of degree 4 and sum of degree 4, *8n + 4m* edges between vertices of sum of degree 4 and sum of degree 5, *30mn + 6n* edges between vertices of sum of degree 5 and sum of degree 5, *60mn + 20n + 4m* edges between vertices of sum of degree 5 and sum of degree 8, *20mn + 12n + 4m* edges between vertices of sum of degree 8 and sum of degree 8, *80mn + 16n* edges between vertices of sum of degree 8 and sum of degree 9, and *59mn – 2n – 15m* edges between vertices of sum of degree 9 and sum of degree 9 for the graph G_L.

We apply this information about edge partitions based on the degree sum of the neighbour vertices of each vertex for graphs G_L and G_{LP} into Formula 6 and obtain the desired results. This completes the proof.

Theorem 4. Let G_L and G_{LP} be the line graph and paraline graph of chemical structures of the conductive 2D MOFs. Then:

$$GA_5(G_L) = \left(\frac{2}{5}\right)(4m+8)\sqrt{6} + \left(\frac{6}{19}\right)(4m+8n)\sqrt{10} + \left(\frac{3}{11}\right)(4m+8n)\sqrt{13} + 48mn - 2m + 2n + \left(\frac{2}{21}\right)(20mn - 4m - 4n)\sqrt{110} + \left(\frac{2}{11}\right)(40mn + 8n)\sqrt{30} + \left(\frac{2}{23}\right)(4m+8n)\sqrt{130} + \left(\frac{1}{12}\right)(4m+8n)\sqrt{143} + \left(\frac{2}{25}\right)(36mn - 8m - 16n)\sqrt{154} + \left(\frac{1}{13}\right)(4mn+4m)\sqrt{165} + \left(\frac{2}{27}\right)(4m+8n)\sqrt{182} + \left(\frac{2}{29}\right)(4mn-4m)\sqrt{210} + \left(\frac{8}{31}\right)(4mn-4m)\sqrt{15},$$

$$GA_5(G_{LP}) = 20n - 9m + \left(\frac{4}{9}\right)(8n+4m)\sqrt{5} + 109mn + \left(\frac{4}{13}\right)(60mn+20n+4m)\sqrt{10} + \left(\frac{12}{17}\right)(80mn+16n)\sqrt{2}.$$

Proof. By applying the same information as in Theorem 4 into Formula 7, we obtain the desired results. This completes the proof.

By using Formulas 8 to 12, we can compute the hyper-Zagreb index, $HM(G)$, the first multiple Zagreb index, $PM_1(G)$, the second multiple Zagreb index, $PM_2(G)$, and the Zagreb polynomials, $M_1(G,x)$ and $M_2(G_L,x)$, for the graphs G_L and G_{LP} in the following theorem. We omit the proof since it is similar to the proofs of Theorems 1 to 4.

Theorem 5. Let G_L and G_{LP} be the line graph and paraline graph of chemical structures of the conductive 2D MOFs. Then:

i. $HM(G_L) = -36m + 228n + 1068mn$,

ii. $HM(G_{LP}) = 7704mn + 1724n - 200m$,

iii. $PM_1(G_L) = 1680(4m + 8n)(50mn + 18n + 4m)(80mn + 16n)(26mn - 10m - 4n)$,

iv. $PM_1(G_{LP}) = 80(30mn + 18n + 6m)(60mn + 4m + 20n)(159mn + 26n - 11m)$,

v. $PM_2(G_L) = 96(30mn + 18n + 6m)(60mn + 4m + 20n)(159mn + 26n - 11m)$,

vi. $PM_2(G_{LP}) = 10368(4m + 8n)(50mn + 18n + 4m)(80mn + 16n)(26mn - 10m - 4n)$,

vii. $M_1(G_L, x) = (4m + 8n)x^5 + (50mn + 18n + 4m)x^6 + (80mn + 16n)x^7 + (26mn - 10m - 4)x^8$,

viii. $M_1(G_{LP}, x) = (30mn + 18n + 6m)x^4 + (60mn + 20n + 4m)x^5 + (159mn + 26n - 11)x^6$,

ix. $M_2(G_L, x) = (4m + 8n)x^6 + (50mn + 18n + 4m)x^9 + (80mn + 16n)x^{12} + (26mn - 10m - 4n)x^{16}$,

x. $M_2(G_{LP}, x) = (30mn + 18n + 6m)x^4 + (60mn + 20n + 4)x^6 + (159mn + 26n - 11m)x^9$.

Conclusions

In this article, we focused on the paraline graph representation of the conductive 2D metal-organic frameworks $Cu_3(HITP)_2\ [m, n]$ and investigated their topological indices. We determined the first general Zagreb index M_α, general Randić connectivity index R_α, general sum-connectivity index χ_α, atom-bond connectivity index ABC, geometric-arithmetic index GA, fourth version of atom-bond connectivity index ABC_4, fifth version of geometric-arithmetic index GA_5, hyper-Zagreb index HM(G), first multiple Zagreb index $PM_1(G)$, second multiple Zagreb index $PM_2(G)$, and Zagreb polynomials $M_1(G, x)$, $M_2(G, x)$.

In the future, we are intrigued by the prospect of designing incipient architectures or networks, and then studying their topological indices, which will be quite useful in understanding their underlying topology.

Acknowledgements

The authors would like to thank the referees for their helpful suggestions, which led to the improvement of the article.

Conflict of Interest Statement

The authors declare no conflict of interest. The funders had no role in the design of the study, in the collection, analysis, or interpretation of data, in the writing of the manuscript, or in the decision to publish the results.

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