COMPUTATION AND ALGORITHMIC SOLUTION OF TOPOLOGICAL INDICES OF CERTAIN GRAPHS

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APRIL 2021

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A solitary number that can be utilized to describe some property of the graph of a particle is known as a topological index for that graph. There are various topological indices that have discovered a few applications in hypothetical science. In this thesis, different topological index are computed, algorithms are devised for complicated computations and also where mathematical computation was not possible. In the first thesis, construction algorithm for zero divisor graph with finite rings is developed. Computer based experiments are conducted to find the properties or characteristics of these graphs. On the basis of those properties further algorithms are developed to compute eccentric topological indices for zero divisor graph. The results of algorithm are compared with mathematical computations. Also, degree based topological indices are computed for line graph and subdivision of line graph of benzene ring in P-type-surface network and conductive two dimensional metallic organic frameworks $Cu_3(HITP)_2[m,n]$. Also, algorithms are developed for distance calculator and distance based topological indices calculations for complete binary tree and complete ternary tree.

Abstrak tesis yang dikemukakan kepada Senat Universiti Malaysia Terengganu sebagai memenuhi keperluan untuk Ijazah Sarjana Sains

PENGIRAAN DAN PENDEKATAN BERALGORITMA BAGI INDEK TOPOLOGI DALAM GRAF

KASHIF ELAHI

APRIL 2021

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Nombor tunggal yang dapat digunakan untuk memerihalkan beberapa sifat graf bagi suatu partikel dikenali sebagai indek topologi bagi graf berkenaan. Terdapat berbagai indek topologi yang mempunyai aplikasi dalam sains hipotetikal. Dalam tesis ini, indek topologi berbeza akan dikira, algoritma akan direka untuk pengiraan yang kompleks and di mana pengiraan bermatematik adalah mustahil ditunjukkan. Dalam permulaan tesis, algoritma pembinaan untuk graf pembahagi sifar dengan gelanggang terhingga akan dibangunkan. Eksperimen berdasarkan komputer akan dijalankan untuk menentukan sifat-sifat atau pencirian bagi graf berkenaan. Atas dasar sifat-sifat tersebut, algoritma lanjutan akan dibangunkan untuk mengira indek topologi eksentrik bagi graf pembahagi sifar. Keputusan beralgoritma akan dibandingkan dengan pengiraan bermatematik. Indek topologi berdasarkan darjah juga akan dikira untuk graf garisan dan sub-pembahagian untuk graf garisan bagi gelanggang benzene dalam jaringan permukaan-jenis-P dan kerangka logam organik berdimensi dua konduktif $Cu_3(HITP)_2[m,n]$. Algoritma juga dibangunkan untuk kalkulator jarak dan indek topologi berdasarkan jarak untuk pokok binari lengkap dan pokok ternari lengkap.

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APPROVAL

I certify that an Examination Committee has met on 17th December 2020 to conduct the final examination of Kashif Elahi, on his Doctor of Philosophy thesis entitled "**Computation and Algorithmic Solution of Topological Indices of Certain Graphs**" in accordance with the regulations approved by the Senate of Universiti Malaysia Terengganu. The Committee recommends that the candidate be awarded the relevant degree. The members of the Examination Committee are as follows:

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APPROVAL

This thesis has been accepted by the Senate of Universiti Malaysia Terengganu as fulfilment of the requirements for the degree of Doctor of Philosophy.

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DECLARATION

I hereby declare that the thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at UMT or other institutions.

KASHIF ELAHI
Date: 11/5/2021

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E	edge set
V	vertex set
$\|V\|$	order of G
$\|E\|$	size of G
d_{x_1}	degree of vertex x_1 (in G)
S_{x_1}	sum of degrees of all vertices adjacent to the vertex x_1
δ, Δ	minimum and maximum degree of G
P_m	path on m vertices
C_m	cycle on m vertices
K_m	complete graph on m vertices
$d(x_1, x_2)$	shortest distance between vertices x_1 and x_2
$K_{m,n}$	complete bipartite graph
G_L	line graph of G
G_{PL}	para line graph of G
R	commutative ring with identity
$Z(R)$	set of zero divisors of R
$G(R)$	zero divisor graph of R
$G \bigcup H$	union of graphs G and H
$G \bigcap H$	intersection of graph G and H
$G \times H$	cartesian product of G and H
$G \bigodot H$	corona product of G and H
T	tree
l	leaves of tree
H	height of tree
DFT	Depth First Traversal
BFT	Breath First Traversal
$W(G)$	Winner index
$R_\alpha(G)$	gerneal Randić index of G
$\chi_\alpha(G)$	general sum-connectivity index of G
$M_\alpha(G)$	general Zagreb index of G
ABC index	atom-bond connectivity index
ABC_4 index	fourth version of ABC index
GA index	geometric-arithmetic index
GA_5 index	fifth version of GA index
$H(G)$ index	Harmonic index

AZI(G)	augmented Zagreb index
RZ(G)	redefined versions of the Zagreb index
$PM_1(G)$	first multiple Zagreb index
$PM_2(G)$	second multiple Zagreb index
$M_1(G, x)$	first Zagreb polynomial
$M_2(G, x)$	second Zagreb polynomial
$\varepsilon(x_1)$	eccentricity of vertex x_1
$\xi(G)$	eccentric connectivity index
$\zeta(G)$	total eccentricity index
$ECP(G, x)$	eccentric connectivity polynomial
$\xi^{ac}(G)$	augmented eccentric connectivity index
$\xi^{C}(G)$	connective eccentric index
$E\zeta(G)$	Ediz eccentric connectivity index
${}^{Re}\zeta(G)$	reverse eccentric connectivity index
$GA_4(G)$	geometric-arithmetic eccentric index
$ABC_5(G)$	atom-bond connectivity eccentric index
$H_4(G)$	fourth type of eccentric harmonic index
$WW(G)$	Hyper-Wiener index
$H(G, x)$	Hosoya polynomial
$Sc(G)$	Schultz index
$Sc^*(G)$	modified Schultz index
$Sc(G, x)$	Schultz polynomial
$Sc^*(G, x)$	modified Schultz polynomial
$\mathbb{Z}_n$	set of positive integers of modulo n
$\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$	commutative rings with $p_2 > p_1$ and q are primes numbers
$\Gamma(\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q)$	zero divisor graph of the commutative rings $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$
$NK(G)$	Narumi-Katayama index

CHAPTER 1

INTRODUCTION

1.1 Introduction

In this chapter, basic terminologies and notations of graphs, trees and algorithms are discussed. Initially graph theory was used to deal with recreational purpose, but gradually this mathematical domain evolved as multi-disciplinary research and development for applied sciences. Graphs can model the situations to resolves different kinds of problems. Applications of graphs in chemistry, physics, robotics, optimizations, computer science, statistics, algorithms have served the mankind a lot as shown in Figure 1.1. In 1736, Königsberg formula related three variables as vertices, edges and faces, $V + E + F = 2$ that was start of combinatorial topology. Trees (a type of graphs) have played a vital role in the field of computer science and networks, as they are used in memory management, compiler construction and software development. Binary search trees are used in the field of data structures.

Topological index is an important graph invariant (a numeric value) represents characteristics of the whole graph. Nowadays, research in the area of topological index is expanding in the field of chemical graph theory, computer networks, physics, robotics, memory management, and statistics. In Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR), topological indices are used to

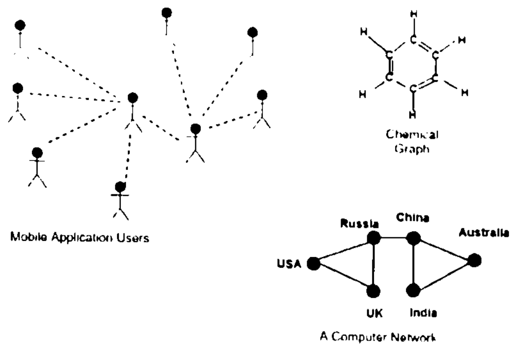


Figure 1.1: Applications of graphs.

determine the organic movements and the atomic properties. Topological indices can be classified in different ways degree based topological indices, distance based topological indices and eccentric topological indices. Wiener index was the first topological index introduced by Harry Wiener in 1947 [93]. A number of topological indices have been introduced including zagreb indices [51], atom bond connectivity [35], geometric arithmetic index [52], randic connectivity index [72], harmonic index [75], sum connectivity index, hosoya index and schultz indices [82].

An algorithm is a well-defined procedure that can be implemented on a computer to solve the problem. They provide a road map for accomplishing a given task, in an accurate and efficient way for any complicated complex computations. The term algorithm belongs to the mathematician of 9th century, Abu Jafer Muhammad Ibn e Musa al-Khawarzmi. Some basic graph algorithms like Dijkstra's, breadth first search (BFS), depth first search (DFS), shortest paths and spanning-tree, Bellman-Ford and Floyd-Warshall algorithms are of great interest to use them in different applications [22].

In this thesis, research is expanded by calculating different types of topological indices on zero divisor graph containing finite rings, line graph and subdivision of line graph of benzene ring, graph, line graph and subdivision of line graph of chemical structures of the conductive two dimensional metallic organic frameworks, complete binary trees and complete ternary trees.

Algorithms are devised for complicated computations. It was complicated to create graphs of large size manually for zero divisor graphs with finite rings, and for complete binary trees, and complete ternary trees mathematical calculation of topological indices was tough. Construction algorithm is devised for zero divisor graph with finite rings. Computer based experiments are conducted to find the properties or characteristics of these graphs. On the basis of those properties further algorithms are devised to compute eccentric topological indices for zero divisor graph. The results of algorithm are compared with mathematical calculations. Degree based topological indices are computed for the graphs of benzene ring and conductive two dimensional metallic organic frameworks. Algorithms are devised for distance calculator and distance based topological indices calculations for complete binary tree and complete ternary tree.

1.2 Graph Terminologies

A *graph* $G = (V, E)$ consists of non-empty set of vertices V and edges E. The number of vertices and edges of graph are known as *order* and *size* of the graph, respectively. If the set V of graph G is finite (infinite) then the graph is *finite (infinite) graph.* Two vertices in an undirected graph are *adjacent* , if these is an edge between them and such edge is known as incident. If more than one edges have same two end points then such edges are called the *multiple edges* and the graph contains multiple edges is known as *multigraphs.* An edge connects to a vertex itself is called *loop.* A graph which does not contain the multiple edges and loops is called *simple graph.* The degree of a vertex x_1 in an undirected graph is number of edges incident to a vertex x_1, except a loop at a vertex x_1 contributes twice to the degree of that vertex, it is denoted by d_{x_1}.

A *path* of length $m - 1$, denoted by P_m, is a sequence of distinct edges

$x_1x_2, x_2x_3, \ldots, x_{m-1}x_m$. A closed path, a path with $x_1 = x_m$, is called a *cycle* or a *circuit*. Figure 1.2 gives example of the cycle C_8 and the path P_8. For any two vertices x_1 and x_2 in graph, the shortest path between them is called *distance* between them and it is denoted by $d(x_1, x_2)$. A *connected graph* G is a graph in which there is a path between every two pair of distinct vertices. Otherwise, a graph is called *disconnected*. A circuit free and connected graph is called a *tree*. A path is a special kind of tree.

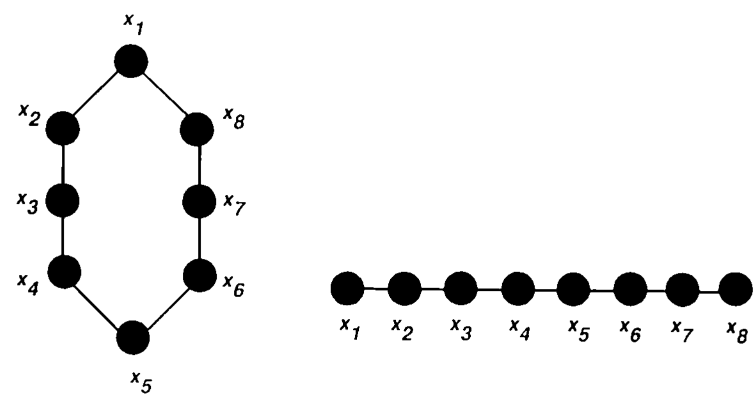


Figure 1.2: Graph of the cycle C_8 and the path P_8.

The maximum distance of a vertex to all other vertices in a graph is called the *eccentricity* of that vertex and the maximum eccentricity of a vertex in a graph is the *diameter* of that graph. The maximum and minimum degree of a graph is denoted by Δ and δ, respectively. Figure 1.3 gives an example of connected graph G, disconnected graph H, the diameter, maximum degree and minimum of graph G is 3,4 and 1, respectively. The eccentricity of vertices x, u, w, z is 3 and y, v is 2.

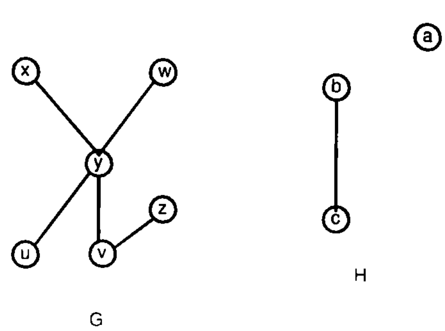


Figure 1.3: Connected graph G and disconnected graph H.

Types of graphs

A *complete graph* is a graph that consists of exact one edge between each pair of vertices. A complete graph of m vertices is denoted by K_m. Figure 1.4 shows examples of complete graphs.

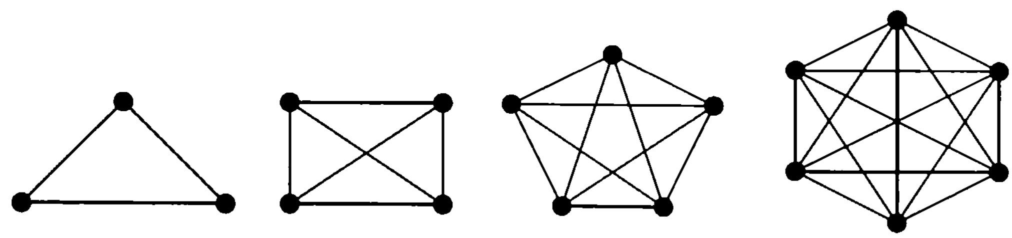


Figure 1.4: Complete graphs.

If the vertex set V of a simple graph G can be partitioned into two disjoint sets X_1 and X_2 such that every edge in the graph connects a vertex in X_1 and a vertex in X_2, then it is called *bipartite* graph. Let the order of the set X_1 is m and set X_2 is n. If all the vertices of set X_1 are connected with all vertices of set X_2, then it is called *complete bipartite* graph, denoted by $K_{m,n}$. Figure 1.5 and Figure 1.6 shows some examples of bipartite and complete bipartite graph.

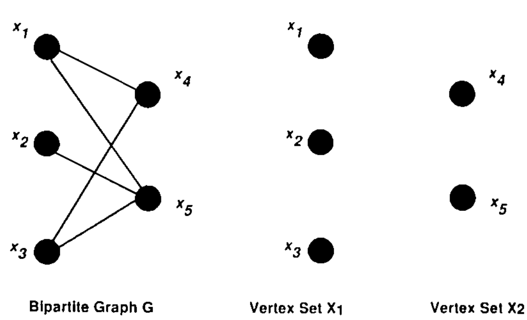


Figure 1.5: Bipartite graphs.

A non-empty set R with two binary operations, addition and multiplication is called a ring. If the multiplication operation is commutative, then the ring is a commutative ring. Let R be a commutative ring with identity and $Z(R)$ is the set of all zero divisors of R. $G(R)$ is said to be a *zero divisor graph* if $x_1, x_2 \in V(G(R)) = Z(R)$ and $(x_1, x_2) \in E(G(R))$ if and only if

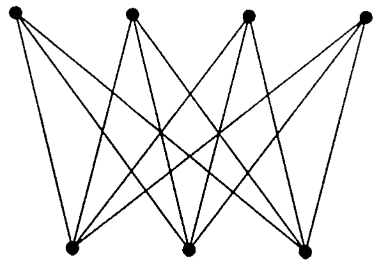


Figure 1.6: Complete bipartite graphs.

$x_1.x_2 = 0$. Beck [14] introduced the notion of zero divisor graph. Figure 1.7. shows a zero divisor graph of $Z(25)$. Where, $Z(25)$ is a set of positive integers of modulo $n = 25$, containing elements $0, 1, 2, 3, 4, 5, 6, ..., 24$. If the remainder from 25, of the product of any two elements of Z is 0, then the elements are adjacent in the zero divisor graph.

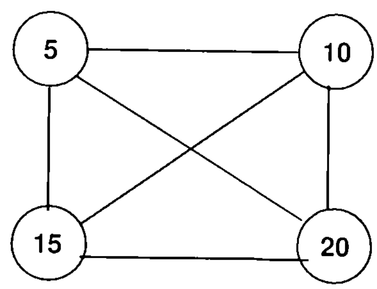


Figure 1.7: Zero divisor graph of $Z(25)$.

A graph of *Benzene ring* refers to the graph of chemical structure that consists of six atoms of carbon, bounded by alternative bounds. In study of chemical structures, benzene ring is represented by C_6H_6. In graph theory, benzene ring is represented by hexagon. Benzene rings are part of many important chemical structure as naphthalene, anthracene, phenanthrene, and pyrene. In Figure 1.8, graph A consists of four benzene rings and graph B consists of 8 benzene rings. Ó Keeffe, Sankey and Adams worked together for low energy forms of carbon [76]. They have distributed around a quarter century a letter managing two 3D systems of benzene one of the structure was called $6.82P$ (additionally polybenzene) and has a place with the space gather $Im3m$ (one of the cubic phase or hexagonal tubular arrangement), comparing to the P-type surface. Actually this is inserting of the hexagon-fix in the surface of negative ebb and flow (phases of tide) P. The P-type surface is coordinated to the Cartesian arranges in the Euclidean space.

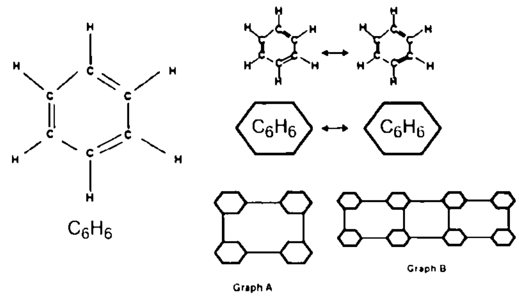


Figure 1.8: Benzene rings.

A graph of *MOFs* or *metallic organic framework* refers to the structure of $Cu_3(HITP)_2(HITP = 2,3,6,7,10,11$ hexaiminotriphenylene). $Cu_3(HITP)_2(HITP = 2,3,6,7,10,11-$hexaiminotriphenylene) is an incipient electrically conductive two dimension metallic organic framework. In recent years, there has been incrementing interest in utilizing metal-organic frameworks (MOFs) as next-generation functional materials in electronic and optoelectronic contrivances. Owing to their high surface area and robust chemical tunability predicated on a "bottom-up" synthetic approach, MOFs have been especially targeted for use in sensors. The utility of metal-organic frameworks (MOFs) as functional materials in electronic contrivances has been inhibited to date by a lack of MOFs that exhibit high electrical conductivity. A *line graph* of a graph G is a graph in which each edge of G represents a vertex and two vertices in line graph are adjacent if and only if their corresponding edges share a common endpoint. Figure 1.9 is representing $Cu_3(HITP)_2(HITP = 2,3,6,7,10,11-$hexaiminotriphenylene) and its line graph.

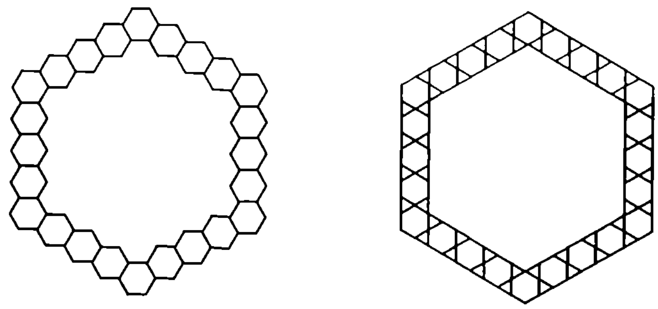


Figure 1.9: The unit cell of graph 2D MOF of $Cu_3(HITP)_2$ and its line graph.

1.2.1 Graph Operations

The *union of two graphs* is simply the union of their vertex and edge sets. If $G = (V_1, E_1)$ and $H = (V_2, E_2)$ are two graphs, then their union is $V_1 \bigcup V_2$ and $E_1 \bigcup E_2$, it is represented by $G \bigcup H$. The *intersection* of two graph $G = (V_1, E_1)$ and $H = (V_2, E_2)$, involves the operation of $V_1 \bigcap V_2$ and $E_1 \bigcap E_2$, it is denoted by $G \bigcap H$. The *join* graph of two graph $G = (V_1, E_1)$ and $H = (V_2, E_2)$, is a union of both graphs with connecting all the vertices of V_1 to V_2 through additional edges.

A *Cartesian product* of two graphs G and H, denoted by $G \times H$, is the graph with vertex set $V(G) \times V(H)$, where two vertices (x_1, y_1) and (x_2, y_2) are adjacent if and only if $x_1 = x_2$ and $y_1 y_2 \in E(H)$ or $y_1 = y_2$ and $x_1 x_2 \in E(G)$.

The *corona product* of two graphs G and H, is the graph obtained by taking one copy of G and $|V(G)|$ copies of H and joining the $i-th$ vertex of G to every vertex in the $i-th$ copy of H [94].

A **subdivision graph** of a graph G is obtained by inserting a vertex on each edges in G. According to the handshaking lemma, in any graph, the sum of degree of all the vertices is equal to twice the number of edges [22]. The vertex partition of a G based on the degree of vertices consists of the degree of vertices and their count. If $e_{u,v}$ denotes the number of edges connecting the vertices of degree d_u and d_v. Then the edge partition of G based on the degree of end vertices of each edge consists of all $e_{u,v} \in E(G)$, and their number of edges. If $m_{i,j}$ denotes the number of edges of G with $i = S_{x_1}$ and $j = S_{x_2}$. Where, S_{x_1} and S_{x_2}, are the summation of degree of neighbor vertices of x_1, and x_2, respectively. Then, the edge partition of graph G based on degree sum of neighbor vertices of end vertices of each edge, will consists of all $m_{i,j}$ in G, their number of edges.

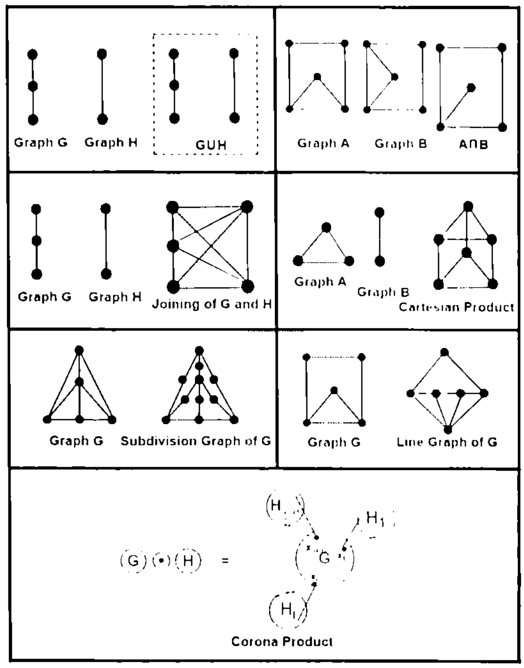


Figure 1.10: Graph operations.

1.3 Tree Terminologies

A. Cayley introduced tree in 1857, while counting the types of some chemical compounds. An undirected connected graph without circuits and loops is called a *tree*. Usually a tree is denoted by T. There are $n - 1$ edges if there are n vertices in a tree T. Nowadays trees are playing an important part in many disciplines, including mathematics, computer sciences, social sciences, chemical sciences, civil networks. They are used in memory management and compiler constructions. They provides solutions for complex problems. In many applications of tree, one vertex is designated as root of the tree. Each edge is directed away from that root. Such a tree is a *rooted tree*. Structure of a rooted tree is based on hierarchical levels. If there exists a direct edge from a vertex u to a vertex v, then u is the *parent* or *ancestor* of v and v is the *child* of u. All the children of vertex u are *descendants*. All the vertices which have same parent vertex are *siblings*. *Root* is a vertex without any parent. The vertices which have no child are *leaf* or *pendant vertex* and represented by l. Any vertex v other than root which have at least one child is called *internal vertex*. In a rooted tree, the length of the unique path from any vertex v to the root is the *height* of that vertex in the tree. All the vertices of height H are at *level* H in the tree. The root is the only vertex with level 0. A rooted tree where children of each internal vertices are ordered is called *ordered rooted tree*. The main purpose of ordered rooted tree is to show children of all the vertices in an order from left to right. Figure 1.11 shows the rooted trees.

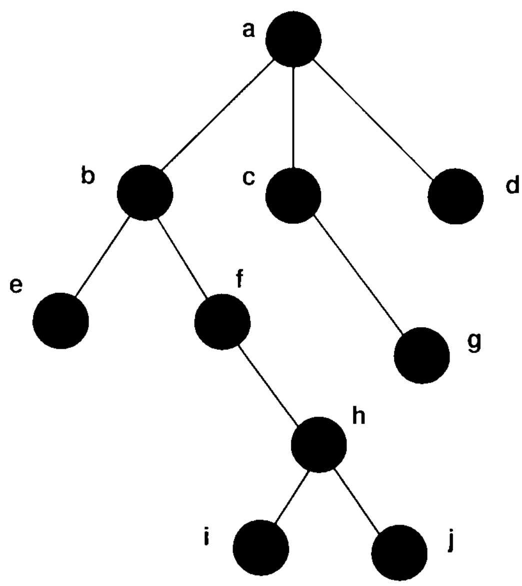


Figure 1.11: Rooted tree.

An *m-ary* tree is a rooted tree with all the internal vertices have maximum m children. The m-ary tree with all internal vertices have exact m children is called *full m-ary* tree. If all leaves are at the same height in a full m-ary tree then it is a *complete m-ary* tree. An m-ary tree with $m = 2$ is called a binary tree. An m-ary tree with $m = 3$ is called a ternary tree. A complete m-ary tree with $m = 2$ and $m = 3$ is called, complete binary tree(CBT) and complete ternary tree(CTT), respectively. Maximum leaves in an m-ary tree can be determined by $l \leq m^H$. The total number of vertices can also be calculated from leave $n = \frac{ml-1}{m-1}$ [81]. In any complete m-ary tree with height the H, the number of vertices are equals to $\frac{m^{H+1}-1}{m-1}$, the degree of root is equals to m, there are m^H leaves which have the degree 1 and $\frac{m^H-m}{m-1}$ internal vertices which have the degree $m+1$. Figure 1.12 shows the binary and ternary tree.

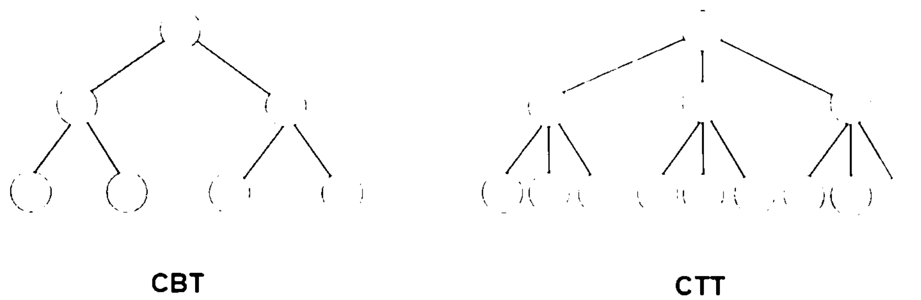
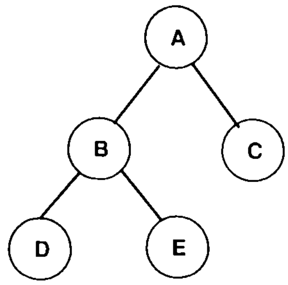


Figure 1.12: Complete Binary tree and Complete Ternary tree.

1.3.1 Tree Traversals

Tree traversal is a systematic procedure or approach to visit each vertex of an ordered rooted tree. Some known tree traversal are preorder traversal, inorder traversal and postorder traversal. If T is an ordered rooted tree with root r. If T have only a single vertex r, then preorder traversal is r. If T consists of sub-trees $T_1, T_2, ..., T_n$ at r from left to right, then preorder traversal starts from r, continues traversing T_1 in preorder, then traversing T_2 in preorder and so on, until completes the traversing of T_n in preorder. If T is an ordered rooted tree with root r. If T have only a single vertex r, then inorder traversal is r. If T consists of sub-trees $T_1, T_2, ..., T_n$ at r from left to right, then inorder traversal starts from T_1, then visits r, continues traversing T_2 in inorder, then traversing T_3 in inorder and so on, until completes the traversing of T_n in inorder. If T is an ordered rooted tree with root r. If T have only a single vertex r, then postorder traversal is r. If T consists of sub-trees $T_1, T_2, ..., T_n$ at r from left to right, then postorder traversal starts from T_1 in postorder, continues traversing T_2 in postorder, and so on, until completes the traversing of T_n in postorder and then visits the root. Figure 1.13 shows an examples of preorder, inorder and postorder traversals.



Inorder	Preorder	Postorder
D B E A C	A B D E C	D E B C A

Figure 1.13: Tree traversal.

1.4 Algorithmic Terminologies

In this section, we define the algorithm designing structures.

1.4.1 Algorithm Design

An algorithm is intended to tackle a specific issue that may belongs to any field of life. Algorithms are frequently used in computing science. Algorithm designing requires a solid scientific and computer science background. Computer based algorithms have solved larger and complex problems of real life with optimality, accuracy, and efficiency.

In algorithm design, exactness and optimality are the key attributes. In any problem, algorithm must provide the required result otherwise it has no use. Algorithm is also unacceptable, if it provides the required result but it is too slow. For algorithm designing, different design architectures, design strategies and data-structures can be used. But for efficient and optimality purpose use of appropriate architecture, strategy and data-structure must be used according to logic of the given problem.

Algorithm Design Architectures

An algorithm design architecture can be iterative or recursive. Iterative design architecture involves loops for repeating a code segment while recursive design architecture call itself again and again to manage repeating instructions. Which design architecture will use in the algorithm is depends on the nature of the problem. In this thesis, construction algorithm for zero divisor graph and algorithm for edge-based eccentric topological indices for zero divisor graph in chapter 3 are designed using iterative approach. In the chapter 5, the algorithm for distance calculation and the algorithm for calculating distance based topological indices for the complete binary and ternary trees use both iterative and recursive architectures according to complex nature of problem, that is explained in detail as algorithm description.

Algorithm Design Strategies

Selection of design strategy is the most technical and crucial task in algorithm designing. Because appropriate design strategy may lead towards accuracy of results and efficiency of the algorithm. Efficiency of an algorithm can be analyzed by measuring its time complexity. Time complexity $T(n)$ of an algorithm means quantification of time taken by an algorithm to produce desired output from given input. T is time and n is size of input data. Algorithms are analyzed on three asymptotic bounds that are known as worst-case analysis $O(n)$, average-case analysis $\theta(n)$ and best-case analysis $\Omega(n)$ [22]. By considering that instructions are executed one after another, with no concurrent operations so each instruction is assigned a unit cost 1. If set of instructions are repeated by loops then the cost of instruction will be multiplied with number of iterations to calculate total cost. If algorithm is designed with recursive approach then $T(n)$ will be formed as a recurrence relation. To solve a recurrence, there exist four techniques named substitution method, recursion tree method, master method and Generating function [70].

A data structure is a data organization, management, and storage format that enables efficient access and modification. More precisely, a data structure is a collection of data values, the relationships among them, and the functions or operations that can be applied to the data. An array is a data structure consisting of a collection of elements (values or variables), each identified by at least one array index or key. The two-dimensional array can be defined as an array of arrays. The 2D-Array is organized as matrices which can be represented as the collection of rows and columns. A Tree-of-Array is a dynamic array data-structure for maintaining an array of separate memory fragments (or "leaves") to store the data elements, unlike simple dynamic arrays which maintain their data in one contiguous memory area.

Design strategy directly effects the algorithm correctness and its efficiency thats why it is an important task. There are number of design strategies available like Brute Force, Divide and Conquer, Decrease and Conquer, Backtracking, Branch and bound, Greedy Algorithm, Dynamic programming, and Genetic Algorithms.

Brute Force is a straightforward approach to solve a problem according to its nature. It is a simplest way to design an algorithm but usually time consuming.

In Divide and Conquer approach original problem is divided into sub-problems as its obvious from its name. Then sub-problems are solved and reunited to compute the result of original problem. Backtracking deals with combinational problems, in which a possible solution is started that satisfies all the required conditions. Then we move to the next level and if that level does not produce a satisfactory solution, we return one level back and start with a new option.

Branch and bound looks for the best solution for a given problem as a whole and once solution is found, it can keep improving the solution. In Greedy method the best available solution is chosen at any moment. It is called greedy because it decides on the basis of current situation rather considering the whole problem, so at the end of total solution result may not be optimal. Dynamic programming works exactly like divide and conquer but dynamic programming reuses the solution of sub-problems many times.

Depth First Traversal (DFT) is a searching algorithm used in traversing the nodes of tree or graph. It starts from the root and moves downward to its child nodes and keeps on moving until reach to pendant (leaf) nodes. DFT algorithm involves Stack (LIFO Architecture) that is why after reaching the leaf node back-tracking process starts to visit the siblings and other descendants of root. Alternatively Breath First Traversal (BFT) another traversing approach works level by level or by visiting the immediate nodes of current node. After visiting all immediate neighbors then it move to next level. BFT involves Queue (FIFO Architecture) to traverse the nodes of graph and tree level by level. Path-Finding, Searching algorithms, Topological Sorting (Scheduling Jobs), Solving Puzzles, Detecting Cycle in a graph are some main applications of DFT and BFT.

In Chapter 3, the algorithm to construct a zero divisor graph and the algorithm to calculate edge-based topological indices for zero divisor graph both have iterative design architecture and Brute Force design strategy. In chapter 5, the algorithm for distance calculator and the algorithm for calculating distance based topological indices for both the complete binary trees and the complete ternary trees are recursive and have Divide and Conquer design strategy.

1.5 Aims and Objectives

To investigate the claims of study research-process carried out in a way that it achieved its objectives to support algorithmic and mathematical solutions of topological indices of certain graphs:

(i) To calculate eccentric topological indices of zero divisor graph.

(ii) To calculate degree based topological indices for line graph of benzene ring in p-type surface, and subdivision of line graph of benzene ring in p-type surface.

(iii) To calculate degree based topological indices for two dimensional metallic frameworks, line graph of two dimensional metallic frameworks, and the subdivision of line graph of two dimensional metallic frameworks.

(iv) To calculate distance based topological indices for complete binary trees and complete ternary trees.

1.6 Research Methodology

This section describes the research method how it is adopted to conclude the final results. In the first step problems were identified with the help of detailed literature review. Real gaps and significant problems are discovered to define the scope of research. In phase of research definition, topological indices of graph are focused. Literature review helped to pose the claims in specific to work on topological indices for zero divisor graphs containing finite ring, benzene rings, two dimensional metallic conductive frameworks, complete binary trees and complete ternary trees. Deductive technique is adopted to conclude the hypothesis.

In the phase of research instrumentation, construction algorithm is devised for zero divisor graphs containing finite ring. By using this algorithm, computer based experiments are conducted for different graph structures. Hypotheses are generated on the basis of assumption that the results of algorithm and empirical experiment will be same. For validation, topological indices will compute from the algorithm, will calculate mathematically as well, and both results will compared. Obtained empirical results used in further algorithms to calculate eccentric topological indices for zero divisor graphs. Results of algorithms are also compared with mathematical calculations and theorems are proved for eccentric topological indices for zero divisor graphs containing finite ring. Line graphs and subdivision of line graphs are reviewed, for benzene rings in P-type surface and two dimension metallic conductive frame works. Assumptions are made by studying graph structure and growths from smaller graphs to larger graphs. Empirical data is collected and theorems are constructed for distance based topological indices for benzene rings in P-type surface and two dimension metallic conductive frame works. For distance based topological indices complete binary trees and complete ternary trees are studied. In a computer based experiment algorithms are executed multiple time by changing the parameter of $m = 2,3$ and similarly for height 2 to 8 for distance calculation. With the help of this algorithm, further algorithms are devised to calculate distance base topological indices for complete binary tree and complete ternary tree.

1.7 Organization of the Thesis

In Chapter 1, basic terminologies and notations of graphs, trees, algorithmic complexity and research objectives are given.

In Chapter 2, concepts and preliminary results on graph topological indices including degree, distance and eccentricity based are explained.

In Chapter 3, eccentric topological indices of zero divisor graphs is computed using computer based algorithms.

In Chapter 4, degree based topological indices are calculated for line graph of benzene ring, line graph by utilizing subdivision of benzene ring, graph of two dimensional metallic framework, line graph of two dimensional metallic organic framework and line graph by utilizing subdivision of two dimensional metallic organic framework.

In Chapter 5, distance calculator and distance based topological indices are computed using computer based algorithms for complete binary trees and for complete ternary trees.

In Chapter 6, conclusions and future works are given to summarize the results.

CHAPTER 2

TOPOLOGICAL INDICES

2.1 Introduction

To identify molecular structures of chemical compound, the molecular graph invariants, called topological indices can be used. Topological indices are designed basically by transforming a molecular graph into a number. The first use of a topological index was made in 1947 by the chemist Harold Wiener. Wiener originally defined his index (W) on trees and studied its use for correlations of physico-chemical properties of alkanes, alcohols, amines and their analogous compounds [93].

Analysis of topological indices for a particular graph helps us to understand graph characteristics, their similarities and their differences with respect to the other graphs. Topological indices guide us that how the chemical structure can further grow and what mathematical operations on the graphs with the help of topological indices can extend multidisciplinary research. Moreover these indices have wide applications in nanotube structures [12, 13] and networks [61]. They have achieved an important place in the field of chemistry, pharmaceutical science, memory managements, complex distance related problems, algorithms and networks.

Depending on the importance of topological indices on a graph, these indices are categorized in three types "degree based topological indices", "distance based topological indices" and "eccentricity based topological indices" of graphs. In this chapter, we discuss the some important types of these indices.

2.2 Degree Based Topological Indices

This section is completely dedicated to managing degree-based topological indices. Before discussing them, we must understand basic graph notations and terminologies, these are already defined in Chapter 1, also these notations and terminologies are followed from the book [81]. A topological index is a number that depicts vital and valuable information about molecular structure. In 1975, the very first degree-based index was introduced by Randić [77]:

$$R_{-\frac{1}{2}}(G) = \sum_{x_1x_2 \in E(G)} \frac{1}{\sqrt{d_{x_1} \times d_{x_2}}} \tag{2.1}$$

The authors [17, 6] independently proposed the general Randić index. For more details of the Randić index see [72]. The general Randić index is defined as

$$R_\alpha(G) = \sum_{x_1x_2 \in E(G)} (d_{x_1} \times d_{x_2})^\alpha, \tag{2.2}$$

where $\alpha \neq 0$ is a real number. If $\alpha = -\frac{1}{2}$, then equation (2.2) is called Randić index which is already defined in equation (2.1). By putting $\alpha = 1$ and $\alpha = -1$, in equation (2.2), we obtain the "second Zagreb index" and the "second modified Zagreb index", respectively.

Zhou *et al.* [96] introduced the general sum-connectivity index $\chi_\alpha(G)$ and defined as

$$\chi_\alpha(G) = \sum_{x_1x_2 \in E(G)} (d_{x_1} + d_{x_2})^\alpha, \tag{2.3}$$

where α is a real number. If $\alpha = -\frac{1}{2}$, $\alpha = 1$ and $\alpha = 2$, then equation (2.2) is known as the sum-connectivity index, the first Zagreb index and hyper-Zagreb index [86], respectively. Gutman and Ghorbani defined Narumi-Katayama index [58] as:

$$NK(G) = \prod_{x_1 \in V(G)} (d_{x_1})^{\alpha} \quad (2.4)$$

Zhong [95] defined the Harmonic index as:

$$H(G) = \sum_{x_1x_2 \in E(G)} \frac{2}{d_{x_1} + d_{x_2}}. \quad (2.5)$$

The general Zagreb index studied in [73] and defined as:

$$M_{\alpha}(G) = \sum_{u \in V(G)} (d_u)^{\alpha}, \quad (2.6)$$

where α is a real number. If $\alpha = 2$, then the equation (2.6) is also known as first Zagreb index. If $\alpha = 3$, then the equation (2.6) is called forgotten topological index (also called F-index), which was introduced by Furtula and Gutman in 2015 [45]. Estrada *et al.* invented *atom-bond connectivity index* which is abbreviated as ABC index [34]. ABC index is of much importance due to its correlation with the thermodynamic properties of alkanes, see [33, 55]. The definition for ABC index is as follows:

$$ABC(G) = \sum_{x_1x_2 \in E(G)} \sqrt{\frac{d_{x_1}+d_{x_2}-2}{d_{x_1} \times d_{x_2}}}. \quad (2.7)$$

The fourth version of ABC index was introduced by Ghorbani and Hosseinzadeh [49] and defined as:

$$ABC_4(G) = \sum_{x_1x_2 \in E(G)} \sqrt{\frac{S_{x_1}+S_{x_2}-2}{S_{x_1} \times S_{x_2}}}, \quad (2.8)$$

where $S_{x_1} = \sum_{x_1x_3 \in E(G)} d_{x_3}$ and $S_{x_2} = \sum_{x_2x_3 \in E(G)} d_{x_3}$. Another important degree based topological index is geometric-arithmetic index which is abbreviated as GA index. It was invented by Vukičević and Furtula [89] and is of much importance due to its application to acyclic, unicyclic and bicyclic molecular graphs [25]. The formal definition of GA index is as follows:

$$GA(G) = \sum_{x_1x_2 \in E(G)} \frac{2\sqrt{d_{x_1} \times d_{x_2}}}{d_{x_1} + d_{x_2}}. \tag{2.9}$$

Recently the fifth version of GA is introduced by Graovac *et al.* [53] and defined as:

$$GA_5(G) = \sum_{x_1x_2 \in E(G)} \frac{2\sqrt{S_{x_1} \times S_{x_2}}}{S_{x_1} + S_{x_2}}. \tag{2.10}$$

Urtula *et al.* [44] introduced an augmented Zagreb index as:

$$AZI(G) = \sum_{x_1x_2 \in E(G)} \left(\frac{d_{x_1} \times d_{x_2}}{d_{x_1} + d_{x_2} - 2} \right)^3. \tag{2.11}$$

Ranjini *et al* [80] defined the redefined versions of the Zagreb indices as follows:

$$RZ(G) = \sum_{x_1x_2 \in E(G)} \left(\frac{d_{x_1} + d_{x_2}}{d_{x_1} \times d_{x_2}} \right)^{\alpha} \tag{2.12}$$

where α is a real number. If $\alpha = 1$, then the equation (2.12) is called first redefined Zagreb index. If $\alpha = -1$, then the equation (2.12) is called second redefined Zagreb index.

In [50], Ghorbani and Azimi defined first multiple Zagreb index $PM_1(G)$ and second multiple Zagreb index $PM_2(G)$ defined as:

$$PM_1(G) = \prod_{x_1x_2 \in E(G)} (d_{x_1} + d_{x_2}). \tag{2.13}$$

$$PM_2(G) = \prod_{x_1x_2 \in E(G)} (d_{x_1} \times d_{x_2}). \tag{2.14}$$

These multiple Zagreb indices are studied for some chemical structures in [18, 32, 56, 71, 85], the first Zagreb polynomial $M_1(G, x)$ and second Zagreb polynomial

$M_2(G, x)$ are defined as:

$$M_1(G, x) = \sum_{x_1x_2 \in E(G)} x^{(d_{x_1} + d_{x_2})}. \quad (2.15)$$

$$M_2(G, x) = \sum_{x_1x_2 \in E(G)} x^{(d_{x_1} \times d_{x_2})}. \quad (2.16)$$

2.3 Eccentricity Based Topological Indices

The distance between two vertices x_1 and x_2 is the length of shortest path between them, it is denoted by $d(x_1, x_2)$. The maximum distance between a vertex x_1 to other vertices in graph is known as the eccentricity of x_1 and mathematical, eccentricity is defined as:

$$\varepsilon(x_1) = max\{d(x_1, x_2) : \forall\ x_2 \in V(G)\}. \quad (2.17)$$

Sharma *et al* [84] introduced the eccentric connectivity index in 1997. The general formula of eccentric connectivity index is defined:

$$\xi(G) = \sum_{x_1 \in V} d_{x_1} \times \varepsilon(x_1) \quad (2.18)$$

where $\varepsilon(x_1)$ is the eccentricity of vertex x_1 in G. Some authors studied the applications and mathematical properties of eccentric connectivity index in [29, 65, 69, 97]. The total eccentricity index is the sum of eccentricity of all the vertex x_1 in G and it was introduced by Farooq and Malik [43], which is defined as:

$$\zeta(G) = \sum_{x_1 \in V} \varepsilon(x_1) \quad (2.19)$$

The *first Zagreb index* of a graph G was studied in [73] based on degrees and a new version of the first Zagreb index based on eccentricities was recently introduced by Ghorbani and Hosseinzadeh [51], as follows:

$$M_1^*(G) = \sum_{x_1 \in V(G)} \varepsilon(x_1)^2. \tag{2.20}$$

The *eccentric connectivity polynomial* is the polynomial version of the eccentric-connectivity index which was introduced by Alaeiyan, Mojarad and Asadpour [4] and some graph operations can be found in [10]. The eccentric connectivity polynomial of a graph G is given by the following formula:

$$ECP(G, x) = \sum_{x_1 \in V(G)} d_{x_1} \times x^{\varepsilon(x_1)}. \tag{2.21}$$

Gupta, Singh and Madan [54] defined the *augmented eccentric connectivity index* of a graph G as follows:

$$\xi^{ac}(G) = \sum_{x_1 \in V(G)} \frac{M(x_1)}{\varepsilon(x_1)}, \tag{2.22}$$

where $M(x_1)$ denotes the product of degrees of all vertices adjacent to the vertex x_1. Some interesting results on augmented eccentric connectivity index are discussed in [23, 28]. Another very relevant and special eccentricity based topological index is *connective eccentric index*. The connective eccentric index was defined by Gupta, Singh and Madan [54] as follows:

$$\xi^{C}(G) = \sum_{x_1 \in V(G)} \frac{d_{x_1}}{\varepsilon(x_1)}. \tag{2.23}$$

Ediz [30, 31] introduced the *Ediz eccentric connectivity index* and *reverse eccentric connectivity index* of graph G, which is used in various branches of sciences, molecular science and chemistry etc. Ediz eccentric connectivity index and reverse eccentric connectivity index are defined by the following formulas:

$$E\zeta(G) = \sum_{x_1 \in V(G)} \frac{S(x_1)}{\varepsilon(x_1)}, \tag{2.24}$$

$$^{Re}\zeta(G) = \sum_{x_1 \in V(G)} \frac{\varepsilon(x_1)}{S(x_1)}. \tag{2.25}$$

where S_{x_1} is the sum of degrees of all vertices adjacent to the vertex x_1 and $\varepsilon(x_1)$ is the eccentricity of x_1. In [51, 90], the authors defined the first and third Zagreb eccentric index as:

$$M_1{}^*(G) = \sum_{x_1x_2 \in E(G)} (\varepsilon(x_1) + \varepsilon(x_2)). \tag{2.26}$$

$$M_3{}^*(G) = \sum_{x_1x_2 \in E(G)} (\varepsilon(x_1) \times \varepsilon(x_2)). \tag{2.27}$$

Ghorbani and Khaki [52] introduced the "geometric-arithmetic eccentric index" defined as:

$$GA_4(G) = \sum_{x_1x_2 \in E(G)} \frac{2\sqrt{\varepsilon(x_1) \times \varepsilon(x_2)}}{\varepsilon(x_1) + \varepsilon(x_2)}. \tag{2.28}$$

Farahani [35] defined the "atom-bond connectivity eccentric index" in 2013 as:

$$ABC_5(G) = \sum_{x_1x_2 \in E(G)} \sqrt{\frac{\varepsilon(x_1) + \varepsilon(x_2) - 2}{\varepsilon(x_1) \times \varepsilon(x_2)}}. \tag{2.29}$$

In [42, 46], Farahani *et al* defined the fourth type of eccentric harmonic index

$$H_4(G) = \sum_{x_1x_2 \in E(G)} \frac{2}{\varepsilon(x_1) + \varepsilon(x_2)}. \tag{2.30}$$

2.4 Distance based Topological Index

Distance is an important graph invariant that has wide applications in computing science and other fields of sciences. Some important distance based topological indices are Wiener index, Hyper-Wiener index, Hosoya polynomial, Schultz and modified Schultz polynomials. In this section, we defined these indices.

In 1947, a chemist Harold Wiener [93] illustrate connection between the physico-chemical properties of organic compounds and the index of their molecular graphs. This index is called the Wiener index and defined as:

$$W(G) = \sum_{x_1 x_2 \in V(G)} d(x_1, x_2) \tag{2.31}$$

Randić [78, 79] introduced the Hyper-Wiener index which is used for for predicting physico-chemical properties of organic compounds and defined as follows:

$$WW(G) = \sum_{x_1 x_2 \in V(G)} \left(d(x_1, x_2) + d(x_1, x_2)^2 \right) \tag{2.32}$$

In 1989, Hosoya [62] introduced the Hosoya polynomial which is defined as:

$$H(G, x) = \sum_{x_1 x_2 \in V(G)} x^{d(x_1, x_2)} \tag{2.33}$$

For detail literature review on applications and properties of Wiener index, Hyper-Wiener index and the Hosoya polynomial for chemical structure see [21, 24, 64, 47, 48].

Schultz [83] introduced a topological index for characterizing alkanes by an integer number. The "Schultz molecular topological index" (MTI) of the graph G is defined as follows:

$$MTI(G) = \sum_{i=1}^{n} [\mathbf{d}(\mathbf{A} + \mathbf{D})]_i \tag{2.34}$$

where A and D are the adjacency and distance matrixes of G of order $n \times n$ and

d is vector of degrees of the vertices of G with order $1 \times n$. For a connected graph G and d_{x_1} the degree of a vertex x_1 in G, the degree distance of G is defined as:

$$DD(G) = \sum_{x_1x_2 \subset V(G)} (d_{x_1} + d_{x_2}) d(x_1, x_2) \tag{2.35}$$

This degree distance index introduced in 1994 by Dobrynin and Kochetova [27] and at the same time by Gutman [57], they named this degree distance index "Schultz index".

Klavžar and Gutman [66] defined the modified Schultz index of G as:

$$Sc^*(G) = \sum_{x_1x_2 \in V(G)} (d_{x_1} \times d_{x_2}) d(x_1, x_2) \tag{2.36}$$

In [57], two topological polynomials of a graph G are defined as:

$$Sc(G, x) = \sum_{x_1x_2 \in V(G)} (d_{x_1} + d_{x_2}) x^{d(x_1, x_2)} \tag{2.37}$$

and

$$Sc^*(G, x) = \sum_{x_1x_2 \in V(G)} (d_{x_1} \times d_{x_2}) x^{d(x_1, x_2)} \tag{2.38}$$

The Schultz index $Sc(G)$ and modified Schultz index $Sc^*(G)$ for a graph G as:

$$Sc(G) = \frac{\partial Sc(G, x)}{\partial x}\bigg|_{x=1} \tag{2.39}$$

$$Sc^*(G) = \frac{\partial Sc^*(G, x)}{\partial x}\bigg|_{x=1} \tag{2.40}$$

Immense work on Schultz polynomials and indices, and other related indices is done in these articles [5, 36, 37, 39, 40, 41].

CHAPTER 3

ECCENTRIC TOPOLOGICAL INDICES FOR GRAPH CONTAINING FINITE RINGS

In this chapter, vertex eccentric topological indices and edge eccentric topological indices are focused for zero divisor graph containing finite rings. Algorithms are devised to calculate correct topological indices and are compared with mathematical calculations.

3.1 Introduction

The maximum distance between a vertex x_1 to other vertices in graph is known as the eccentricity of x_1 and mathematical, eccentricity is defined as:

$$\varepsilon(x_1) = max\{d(x_1, x_2) : \forall\ x_2 \in V(G)\}. \tag{3.1}$$

In 1997 eccentric connectivity index was introduced by Sharma [84], he was studying the structure of piperidinyl methyl ester and methylene methyl ester analogs as analgesic agents. By using eccentric connectivity index, the mathematical modeling of biological activities of diverse nature is done. The general formula of eccentric connectivity index is defined in equation (2.18). Farooq and Malik introduced total eccentricity index while working on eccentricity based topological indices of nanostar dendrimers [43], which is defined in equation (2.19).

In 2012, Ghorbani and Hosseinzadeh [51] introduced a new version first Eccentric Zagreb index which is defined in equation (2.20). In equation (2.21), the eccentric connectivity polynomial was proposed by Alaeiyan, Mojarad and Asadpour [4] and Gupta, Singh and Madan [54] defined the augmented eccentric connectivity index in equation (2.22), they also defined another very relevant and special eccentricity based topological index, connective eccentric index in equation (2.23). In equations (2.24) and (2.25), Ediz introduced the Ediz eccentric connectivity index [33] and reverse eccentric connectivity index [30] of graph G.

Let R be a commutative ring with identity and $Z(R)$ is the set of all zero divisors of R. $G(R)$ is said to be a zero divisor graph if $x, y \in V(G(R)) = Z(R)$ and $(x, y) \in E(G(R))$ if and only if $x.y = 0$. Beck [14] introduced the notion of zero divisor graph. Anderson and Livingston [8] proved that $G(R)$ is always connected if R is commutative. Anderson and Badawi [7] introduced the total graph of R as there is an edge between any two distinct vertices $u, v \in R$ if and only if $u + v \in Z(R)$. For a graph G, the concept of graph parameters have always a high interest. Numerous authors briefly studied the zero-divisor and total graphs extracted from commutative rings [3, 9, 11, 15, 16, 82, 87].

Let p_1, p_2 and q are prime numbers, with $p_2 > p_1$. and $\Gamma(\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q)$ be zero divisor graph of the commutative rings $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$. In this chapter, we investigate the eccentric topological descriptors namely, eccentric connectivity index, total eccentric index, first Zagreb eccentricity index, connective eccentric index, Ediz eccentric index, eccentric connectivity polynomial and augmented eccentric connectivity index of zero divisor graphs $\Gamma(\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q)$. Now onward in this chapter, we use G as a zero divisor graph of the commutative rings $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$.

3.2 Construction Algorithm for Zero Divisor Graph

We adopted interdisciplinary methods by combining algorithmic approach for graph construction and outcome of algorithm are aligned with eccentric topological indices. For prime numbers p_1, p_2, q with $p_2 > p_1$, we consider the commutative ring $R = \mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$ with usual addition and multiplication. The zero divisor graph $G = \Gamma(\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q)$ associated with ring R is defined as: For $a \in \mathbb{Z}_{p_1p_2}$, $b \in \mathbb{Z}_q$, $(a,b) \notin V(G)$ if and only if $a \neq kp_1, a \neq sp_2$ for $k = 1, 2, \cdots, p_2 - 1, s = 1, 2, \cdots, p_1 - 1$ and $b \neq 0$. Let $J = \{(a,b) \notin V(G) : a \neq kp_1, a \neq sp_2, k = 1, 2, \cdots, p_2 - 1, s = 1, 2, \cdots, p_1 - 1 \;\&\; b \neq 0\}$, then $|J| = (p_1p_2 - p_1 - p_2 + 1)(q - 1)$. The elements of the set J are the non zero divisors of R. Also $(0, 0) \in \mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$ is a non zero divisor. Therefore, $|J| + 1 = (p_1p_2 - p_1 - p_2 + 1)(q - 1) + 1$ are the total number of non zero divisors of R and the total number of elements of R are p_1p_2q. Hence, $p_1p_2q - (p_1p_2 - p_1 - p_2 + 1)(q - 1) + 1 = (p_1 + p_2 - 1)(q - 1) + p_1p_2 - 1$ are the total number of zero divisors. This implies that $|V(G)| = (p_1 + p_2 - 1)(q - 1) + p_1p_2 - 1$. We can construct the zero divisor graph of commutative ring $R = \mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$ by the following algorithm as:

Algorithm 1 ZeroDivisorGraph(p1,p2,q)

Input: p1,p2 and q are three prime numbers.
Output: ordered pairs for zero divisor.

```
if (p1 < p2)
    for x1 ← 0 to p1 × p2
        for y1 ← 0 to q
            if (x1 ≠ 0 OR y1 ≠ 0)
                createGraph(x1 , y1, p1, p2, q)
```

Algorithm 2 createGraph (x1, y1, p1, p2, q)

```
1:  for x2 ← x1 to p1 × p2
2:     for y2 ← y1 to q
3:        if (x1 ≠ x2 AND y1 ≠ y2)
4:           if (x1 ≠ 0 OR x2 ≠ 0)
5:              k1 = 0
6:           else
7:              k1 = x1 × x2
8:           if (y1 ≠ 0 OR y2 ≠ 0)
9:              k2 = 0
10:          else
11:             k2 = y1 × y2
12:          if (k1 mod p1 = 0 AND k1 mod p2 = 0 AND k2 = 0)
13:             return x1,y1,x2,y2
```

Algorithm Description

Algorithm 1: ZeroDivisorGraph is a construction algorithm for zero divisor graph from primes p_1,p_2 and q. It requires, the three input parameters p_1,p_2 and q to execute. Line 1 in the algorithm just check the basic condition i.e, p_1 must be greater than p_2. Line 2-4, execute nested for-loops. These loops create all possible combinations of a and b coordinates for any vertex v other than both x_1 and y_1 equals to 0, such that x_1 may vary from 0 to $p_1 \times p_2$ and y_1 may vary from 0 to q. Line 5, in the nested loop call createGraph algorithm for all the x_1 and y_1 combinations. The collective running time of Algorithm 1, and the Algorithm 2 is $O(p_1 p_2 q)$.

Algorithm 2: createGraph requires x_1,y_1,p_1,p_2,q parameters to execute. For any vertex having coordinates x_1, y_1, this part finds the connecting vertex u coordinates x_2, y_2. Line 1-2, execute nested for-loops. These loops create all possible combinations of x_2 and y_2 coordinates for any vertex u, such that x_2 may vary from x_1 to $p_1 \times p_2$ and y_2 may vary from y_1 to q. Line 3, apply the condition to omit the edges that create self loops in the graph. Line 4-7, assign k_1 the product of x_1 and x_2. Line 8-11, assign k_2 the product of y_1 and y_2. Line 12-13, ensures the conditions for zero divisor and return the ordered pairs of adjacent vertices, (x_1, y_1) and (x_2, y_2) .

3.2.1 Computer Based Experiments

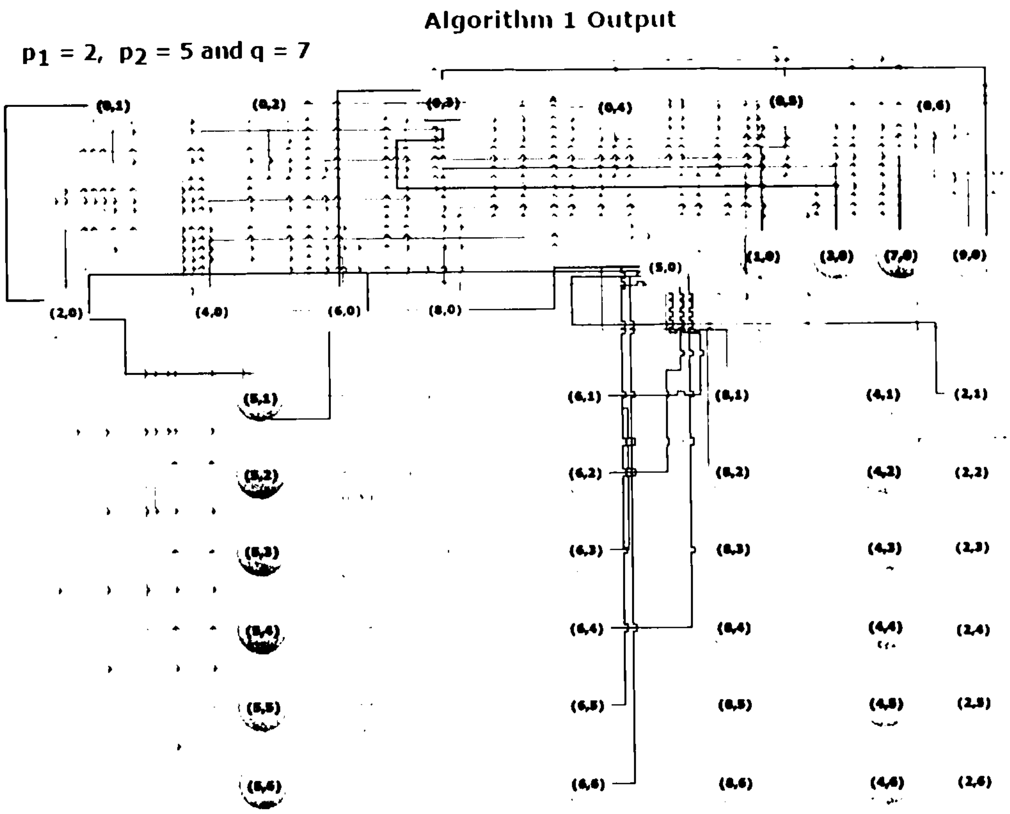


Figure 3.1: Graph generated by experimenting Algorithm 1.

Algorithm 1 has been implemented in computer. A number of zero divisor graphs has been generated from different prime numbers, one of which is shown in the Figure 3.1. Zero divisor graph for $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$ with $p_1 = 2$, $p_2 = 5$, and $q = 7$ has been generated. We found six different partitions of vertices and their adjacencies, the maximum eccentricity 3 and the minimum eccentricity 2. After analyzing these graphs, mathematical properties has been found out.

Outcomes of above algorithm, the degree of each vertex $(a, b) \in V(G)$ can be depicted mathematically in the following cases:

Case 1: If $a = 0$ and any $b \in \mathbb{Z}_q \setminus \{0\}$, then each such type of vertex $(0, b)$ is adjacent to the vertices $(a', 0)$ for every $a' \in \mathbb{Z}_{p_1p_2} \setminus \{0\}$. Hence the degree of each vertex $(0, b)$ is $p_1p_2 - 1$.

Case 2: If $a = kp_1, k = 1, 2, \cdots, p_2 - 1$ and $b = 0$, then each such type of vertex $(a, 0)$ is adjacent to the vertices $(0, b), (a', 0)$ & (a', b') for every $b' = \{1, 2, \cdots, q - 1\}$, and $a' = sp_2, s = 1, 2, \cdots, p_1 - 1$. Hence the degree of each vertex $(a, 0)$ is $q - 1 + p_1 - 1 + (p_1 - 1)(q - 1) = p_1q - 1$. Similarly, if $a = sp_2, s = 1, 2, \cdots, p_1 - 1$ and $b = 0$, then degree of each such type of vertices $(a, 0)$ is $p_2q - 1$.

Case 3: If $a \in \mathbb{Z}_{p_1p_2} \setminus \{0, kp_1, sp_2$ with $k = 1, 2, \cdots, p_2 - 1$, $s = 1, 2, \cdots, p_1 - 1\}$ and $b = 0$, then each such type of vertex $(a, 0)$ is adjacent with only $(0, b')$ for every $b' \in \mathbb{Z}_q \setminus \{0\}$. Hence the degree of each vertex $(a, 0)$ is $q - 1$.

Case 4: If $a = kp_1, k = 1, 2, \cdots, p_2 - 1$ and $b \in \mathbb{Z}_q \setminus \{0\}$, then each such type of vertex (a, b) is adjacent with only $(a', 0)$ for every $a' = sp_2, s = 1, 2, \cdots, p_1 - 1$. Therefore, the degree of each vertex (a, b) is $p_1 - 1$. Similarly, if $a = sp_2, s = 1, 2, \cdots, p_1 - 1$ and $b \in \mathbb{Z}_q \setminus \{0\}$, then degree of each such type of vertices (a, b) is $p_2 - 1$.

From the above discussion, let us partition the vertex set of G based on their degrees as follows:

$$V_1 = \{(0, x) : x \in \mathbb{Z}_q, x \neq 0\}$$

$$V_2 = \{(x, 0) : x = kp_1, k = 1, 2, \ldots, p_2 - 1\}$$

$$V_3 = \{(x, 0) : x = sp_2, s = 1, 2, \ldots, p_1 - 1\}$$

$$V_4 = \{(x, 0) : x \in \mathbb{Z}_{p_1 p_2} \setminus \{0\}, x \neq kp_1, x \neq sp_1, k = 1, 2, \ldots, p_2 - 1,$$
$$s = 1, 2, \ldots, p_1 - 1\}$$

$$V_5 = \{(x, y) : x = kp_1, k = 1, 2, \ldots, p_2 - 1, y \in \mathbb{Z}_q \setminus \{0\}\}$$

$$V_6 = \{(x, y) : x = sp_2, s = 1, 2, \ldots, p_1 - 1, y \in \mathbb{Z}_q \setminus \{0\}\}$$

This shows that $V(G) = V_1 \cup V_2 \cup V_3 \cup V_4 \cup V_5 \cup V_6$. It is easy to see that $|V_1| = q-1$, $|V_2| = p_2-1$, $|V_3| = p_1-1$, $|V_4| = (p_1-1)(p_2-1)$, $|V_5| = (p_2-1)(q-1)$ and $|V_1| = (p_1-1)(q-1)$.

3.3 Main Results for Vertex-based Topological Indices

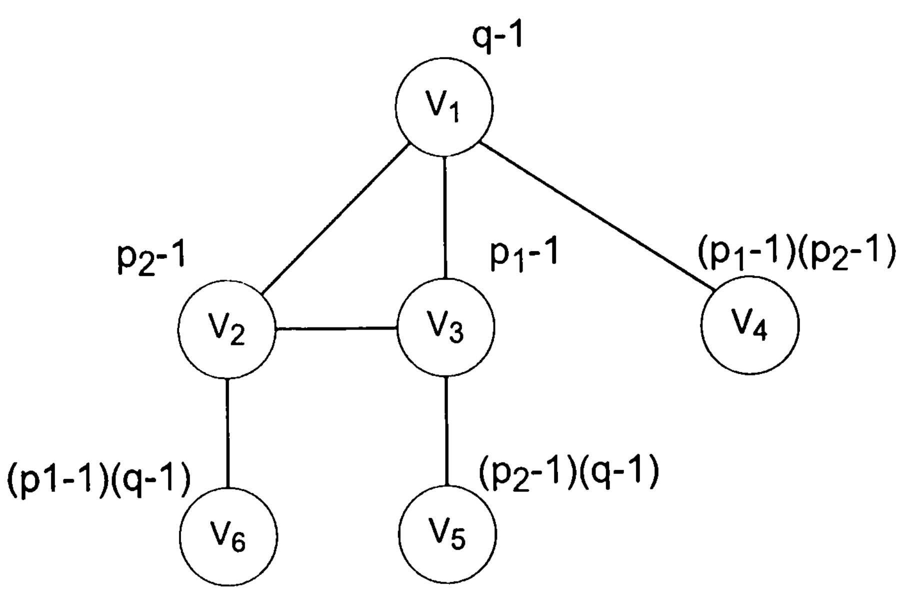


Figure 3.2: Different partitions found in graph generalizing for p_1,p_2,q primes.

Different vertex partitions found in graph can generalize for p_1, p_2, and q primes as shown in Figure 3.2. We have six different vertex partitions V_1, V_2, V_3, V_4, V_5, and V_6. The vertex partition V_1 is adjacent to V_2, V_3, and V_4. The vertex partition V_5 is adjacent to V_3, and the vertex partition V_6 is adjacent to V_2. The eccentricity of the partitions V_1, V_2, and V_3 is 2, and the eccentricity of the partitions V_4, V_5, and V_6 is 3. The cardinality of the partitions V_1 is $(q-1)$, V_2 is (p_2-1), V_3 is (p_1-1), V_4 is $(p_1-1)(p_2-1)$, V_5 is $(p_1-1)(q-1)$, and V_6 is $(p_2-1)(q-1)$.

Let $d_U(u)$ denotes the degree of a vertex u in U and $d(U,V)$ denotes the distance between the vertices of two sets U and V. In the following theorem, we determined the eccentricity of the vertices of G.

Theorem 3.3.1. *Let G be the zero divisor graph of the commutative ring R, then the eccentricity of the vertices of G is 2 or 3.*

Proof. From case 1, the vertices of the set V_1 are at distance 1 with the vertices of the sets V_2 V_3 & V_4 i.e $d(V_1,V_2) = d(V_1,V_3) = d(V_1,V_4) = 1$. From Case 4, the vertices of the sets V_2 and V_3 are adjacent with the vertices of the sets V_6 and V_5, respectively. This implies that $d(V_1,V_5) = d(V_1,V_6) = 2$. The distance between any two different vertices of the set V_1 is also 2. Therefore the eccentricity of the vertices of set V_1 is 2 i.e $e(V_1) = 2$. Similarly, it is easy to see that $e(V_2) = e(V_3) = 2$.

As $d(V_1,V_2) = d(V_1,V_3) = d(V_1,V_4) = 1$ and $d(V_1,V_5) = d(V_1,V_6) = 2$. This implies that $d(V_4,V_5) = d(V_4,V_1)+d(V_1,V_5) = 3$. This shows that $e(V_4) = 3$. Similarly, it is easy to calculate that $e(V_5) = e(V_6) = 3$. This completes the proof. □

Summarizing the above cases, partition of vertices and their cardinality of Theorem 3.3.1 are shown in Table 3.1.

Table 3.1: The representation of vertices, their degree, eccentricity and frequency of the vertices in G.

Representatives of vertices	Degree	Eccentricity	Frequency
V_1	$p_1p_2 - 1$	2	$q - 1$
V_2	$p_1q - 1$	2	$p_2 - 1$
V_3	$p_2q - 1$	2	$p_1 - 1$
V_4	$q - 1$	3	$(p_1 - 1)(p_2 - 1)$
V_5	$p_1 - 1$	3	$(p_2 - 1)(q - 1)$
V_6	$p_2 - 1$	3	$(p_1 - 1)(q - 1)$

In the following theorem, we determine the eccentric connectivity index of the graph G.

Theorem 3.3.2. *Let $p_1 < p_2$, q be prime numbers, then eccentric connectivity index of graph G is $\xi(G) = p_1p_2(15q - 11) - (p_1 + p_2)(11q - 7) + 7q - 3$.*

Proof. By using the degree of each vertex partition and corresponding their eccentricity from Table 3.1 in the equation (2.18), we obtain

$$\xi(G) = \sum_{x_1 \in V} d_{x_1}\, \varepsilon(x_1)$$

$$=2(p_1p_2 - 1)(q - 1) + 2(p_1q - 1)(p_2 - 1) + 2(p_2q - 1)(p_1 - 1)$$

$$+3(p_1 - 1)(p_2 - 1)(q - 1) + 3(p_1 - 1)(p_2 - 1)(q - 1)$$

$$+ 3(p_1 - 1)(p_2 - 1)(q - 1)$$

After simplification, we get

$$\xi(G) = p_1p_2(15q - 11) - (p_1 + p_2)(11q - 7) + 7q - 3.$$

This completes the proof. □

The eccentricity of the vertices of graph G and their frequency is given in Table 3.1, by putting these values and after simplification, we obtain the following two corollaries.

Corollary 3.3.1. *Let $p_1 < p_2$, q be prime numbers, then total-eccentricity index of G is given by $\zeta(G) = 3(p_1p_2 + p_1q + p_2q + 1) - 4(p_1 + p_2 + q)$.*

Corollary 3.3.2. *Let $p_1 < p_2$, q be prime numbers, then the first Zagreb eccentricity index of G is given by $M_1{}^*(G) = 9(p_1p_2 + p_1q + p_2q) - 14(p_1 + p_2 + q) + 15$.*

Theorem 3.3.3. *Let $p_1 < p_2$, q be prime numbers, then connective eccentric index of graph G is $\xi^C(G) = (p_1 - 1)(p_2 - 1)(q - 1) + 2 + \frac{p_1p_2(3q-1)-(p_1+p_2+1)(q+1)}{2}$.*

Proof. By using the values of degrees and their eccentricity in the equation (2.23), we obtain the following:

$$
\begin{aligned}
\xi^C(G) =& \sum_{x_1 \in V} \frac{d_{x_1}}{\varepsilon(x_1)} \\
=& \frac{(p_1p_2-1)(q-1)}{2} + \frac{(p_1q-1)(p_2-1)}{2} + \frac{(p_2q-1)(p_1-1)}{2} \\
+& \frac{(p_1-1)(p_2-1)(q-1)}{3} + \frac{(p_1-1)(p_2-1)(q-1)}{3} \\
+& \frac{(p_1-1)(p_2-1)(q-1)}{3} \\
=& (p_1-1)(p_2-1)(q-1) + 2 + \frac{p_1p_2(3q-1)-(p_1+p_2+1)(q+1)}{2}.
\end{aligned}
$$

After simplification, we obtain

$$
\xi^C(G) = (p_1-1)(p_2-1)(q-1) + 2 + \frac{p_1p_2(3q-1)-(p_1+p_2+1)(q+1)}{2}.
$$

This completes the proof. □

Theorem 3.3.4. *Let $p_1 < p_2$, q be prime numbers, then Ediz eccentric connectivity index of graph G is* $E\zeta(G) = \frac{9(p_1-1)(p_2-1)(q-1)+8[(p_1-1)(p_2q-1)+(p_2-1)(p_1q-1)+(p_1p_2-1)(q-1)]}{6}$.

Proof. S_{x_1} is the sum of degrees of all vertices x_2 which are adjacent to vertex x_1. Calculate the values of S_{x_1} with the help of Table 3.1. Also the eccentricity of each vertex is given in Table 3.1. Putting these vales in equation (2.24), we obtain the followings:

$$\begin{aligned}E\zeta(G) &= \sum_{x_1 \in V(G)} \frac{S_{x_1}}{\varepsilon(x_1)}\\ &= \frac{(p_1-1)(p_2-1)(q-1)+(p_1-1)(p_2q-1)+(p_2-1)(p_1q-1)}{2}\\ &+ \frac{(p_1-1)(p_2-1)(q-1)+(p_1-1)(p_2q-1)+(q-1)(p_1p_2-1)}{2}\\ &+ \frac{(p_1-1)(p_2-1)(q-1)+(p_2-1)(p_1q-1)+(q-1)(p_1p_2-1)}{2}\\ &+ \frac{(q-1)(p_1p_2-1)}{3} + \frac{(p_1-1)(p_2q-1)}{3} + \frac{(p_2-1)(p_1q-1)}{3}\end{aligned}$$

After simplification, we obtain

$E\zeta(G) = \frac{9(p_1-1)(p_2-1)(q-1)+8[(p_1-1)(p_2q-1)+(p_2-1)(p_1q-1)+(p_1p_2-1)(q-1)]}{6}$.

This completes the proof. □

Theorem 3.3.5. *Let $p_1 < p_2$, q be prime numbers, then eccentric connectivity polynomial of graph G is* $ECP(G,x) = (3p_1p_2q - p_1p_2 - p_1q - p_1 - p_2q - p_2 - q + 3)x^2 + 3(p_1-1)(p_2-1)(q-1)x^3$.

Proof. By using the degree of each vertex partition and corresponding their eccentricity from the Table 3.1 in the equation (2.21), we obtain

$$
\begin{aligned}
ECP(G,x) &= \sum_{x_1\in V} d_{x_1} x^{\varepsilon(x_1)} \\
&= (p_1p_2-1)(q-1)x^2+(p_1q-1)(p_2-1)x^2+ \\
&\quad (p_2q-1)(p_1-1)x^2+(p_1-1)(p_2-1)(q-1)x^3+ \\
&\quad (p_1-1)(p_2-1)(q-1)x^3+(p_1-1)(p_2-1)(q-1)x^3 \\
&= (3p_1p_2q-p_1p_2-p_1q-p_1-p_2q-p_2-q+3)x^2+ \\
&\quad 3(p_1-1)(p_2-1)(q-1)x^3.
\end{aligned}
$$

After simplification, we obtain

$$
\begin{aligned}
ECP(G,x) &= (3p_1p_2q-p_1p_2-p_1q-p_1-p_2q-p_2-q+3)x^2+ \\
&\quad 3(p_1-1)(p_2-1)(q-1)x^3.
\end{aligned}
$$

This completes the proof. □

Theorem 3.3.6. *Let $p_1 < p_2$, q be prime numbers, then augmented eccentric connectivity index of graph G is*

$$\xi^{ac}(G) = \frac{(p_1-1)(p_2-1)(p_1p_2-1)^{q-1}+(p_1-1)(q-1)(p_1q-1)^{p_2-1}+(p_2-1)(q-1)(p_2q-1)^{p_1-1}}{3}$$

$$+\frac{(p_1-1)^{p_2q-q-p_2+2}(p_1q-1)^{p_2-1}(p_1p_2-1)^{q-1}+(p_2-1)^{p_1q-p_1-q+2}(p_1p_2-1)^{q-1}(p_2q-1)^{p_1-1}}{2}$$

$$+\frac{(q-1)^{p_1p_2-p_1-p_2+2}(p_1q-1)^{p_2-1}(p_2q-1)^{p_1-1}}{2}.$$

Proof. $M(v)$ is the product of degrees of all vertices u which are adjacent to vertex v. Calculate the values of $M(v)$ with the help of Table 3.1. Also the eccentricity of each vertex is given in Table 3.1. Putting these vales in equation

(2.22), we obtain

$$
\begin{aligned}
\xi^{ac}(G) &= \sum_{x_1 \in V} \frac{M_{x_1}}{\varepsilon(x_1)} \\
&= \frac{(p_1-1)(p_2-1)(p_1p_2-1)^{q-1}}{3} + \frac{(p_1-1)(q-1)(p_1q-1)^{p_2-1}}{3} \\
&+ \frac{(p_2-1)(q-1)(p_2q-1)^{p_1-1}}{3} \\
&+ \frac{(p_1-1)(p_1-1)^{(p_1-1)(q-1)}(p_1q-1)^{p_2-1}(p_1p_2-1)^{q-1}}{2} \\
&+ \frac{(p_2-1)(p_2-1)^{(p_2-1)(q-1)}(p_1p_2-1)^{q-1}(p_2q-1)^{p_1-1}}{2} \\
&+ \frac{(q-1)(q-1)^{(p_1-1)(p_2-1)}(p_1q-1)^{p_2-1}(p_2q-1)^{p_1-1}}{2}
\end{aligned}
$$

After simplification, we obtain the result as desired. □

3.4 Edge-based eccentricity

Edge-based eccentricity indices involved edges rather then vertex in calculations. As an analogy with the first and the second Zagreb indices, Vukičević and Graovac [90] and Ghorbani and Hosseinzadeh [51] introduced two types of Zagreb eccentricity indices that are defined as in equations (2.26) and (2.27). In 2010, Ghorbani and Khaki [52] defined the geometric-arithmetic eccentric index $GA_4(G)$ in equation (2.28) and atom-bond connectivity eccentric index $ABC_5(G)$ was defined by Farahani [35] in equation (2.29). In 2017, Farahani et al. [42] while working on harmonic indices of certain nanotubes, defined the fourth type of eccentric harmonic index $H_4(G)$ which is defined in equation (2.30).

Algorithm 3 calculateTopologicalIndices (a, b, c)

Input: Three prime numbers a, b and c.

Output: Edge-based eccentric topological indices.

1: createGraphSets (a,b,c)
2: $firstZagreb \leftarrow 4 \times EccEdges1 + 5 \times EccEdges2$
3: $thirdZagreb \leftarrow 4 \times EccEdges1 + 6 \times EccEdges2$
4: $GA \leftarrow 2 \times EccEdges1 + 2 \times \sqrt{6/5} \times EccEdges2$
5: $ABC5 \leftarrow \sqrt{1/2} \times EccEdges1 + \sqrt{1/2} \times EccEdges2$
6: $harmonic \leftarrow 1/2 \times EccEdges1 + 2/5 \times EccEdges2$
7: **return** $firstZagreb, thirdZagreb, GA, ABC5, harmonic$

3.4.1 Algorithms for Edge-based Eccentric Topological Indices

3.4.2 Algorithms Description

Algorithm 3: calculateTopologicalIndices requires, the three input parameters a, and c to execute. Line 1 executes createGraphSets algorithm for the input parameters. Line 2-6, calculates edge eccentric topological indices. Line-7 return the edge eccentric topological indices. The collective running time of Algorithm 3, and the Algorithm 4 is $O(p_1 p_2 q)$.

Algorithm 4: createGraphSets is designed on the basis of mathematical properties(already discovered in this chapter). Line 1-2, execute nested for-loops. These loops create all possible combinations of i and j coordinates for vertex v. Line 3-28 in for-loops, calculate the size of vertex sets(V_1,V_2,..,V_6) stated in previous section), by analyzing each vertex. Line 29-34, calculate size of two types of edges by using size of vertex sets, one with eccentricity 2 and the other one with eccentricity 3. The outcome of this algorithm further used by calculateTopologicalIndices to calculate edge eccentric topological indices.

Algorithm 4 createGraphSets (a,b,c)

Input: Three prime numbers a, b and c.

Output: All possible vertex sets of zero divisor graph with eccentricity of each set.

```
for i ← 0 to a × b
  for j ← 0 to c
    if (i ≠ 0 OR j ≠ 0)
     if (a ≠ b)
        if (i mod a ≠ 0 AND i mod b ≠ 0 AND i ≠ 0 AND j = 0)
           D[di] ← AddPoint(i, j)
        else if (i = 0 AND j ≠ 0)
           A[ai] ← AddPoint(i, j)
        else if (i mod a = 0)
           if (j = 0)
              B[bi] ← AddPoint(i, j)
           else
              E[ei] ← AddPoint(i, j)
        else if (i mod b = 0)
           if (j ≠ 0)
              F[fi] ← AddPoint(i, j)
           else
              C[ci] ← AddPoint(i, j)
     else
        if (i mod a ≠ 0 AND i ≠ 0 AND j = 0)
           D[di] ← AddPoint(i, j)
        else if (i = 0 AND j ≠ 0)
           A[ai] ← AddPoint(i, j)
        else if (i mod a = 0)
           if (j = 0)
              B[bi] ← AddPoint(i, j)
           else
              C[ci] ← AddPoint(i, j)
if (a ≠ b)
      EccEdges1 ← ai × bi + ai × ci + bi × ci
      EccEdges2 ← ai × di + bi × fi + ci × ei
else
      EccEdges1 ← ai × bi
      EccEdges2 ← ai × di + bi × ci
return EccEdges1, EccEdges2
```

3.4.3 Verification of Algorithmic Results for Edge-based Eccentric Topological Indices

For any two positive integers a and b, where $G(R)$ be a zero divisor graph containing commutative ring $R = \mathbb{Z}_a \times \mathbb{Z}_b$ with vertex set $V(G(R))$ and edge set $E(G(R))$ then $V(G(R)) = \{(x, y) \in R : x|a \text{ or } y|b \text{ or } x = 0 \text{ or } y = 0\} \setminus \{(0, 0)\}$ and $E(G(R)) = \{((x_1, y_1), (x_2, y_2)) \in V(G(R)) \times V(G(R)) : (x_1x_2, y_1y_2) = (0, 0) \text{ in } R\}$.

Case 1: $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$

For $a = p^2$ and $b = q$, where p, q are prime numbers. Let G_1 be a zero divisor graph containing commutative ring $R = \mathbb{Z}_{p^2} \times \mathbb{Z}_q$. From [2], we obtain $V_t(G_1)$ with $t = p - 1, q - 1, p^2 - 1, pq - 2$ and $| V_{p-1} | = (p - 1)(q - 1)$, $| V_{q-1} | = p(p - 1)$, $| V_{p^2-1} | = q - 1$, $| V_{pq-2} | = p - 1$. By hand shaking lemma $|E(G_1)| = \frac{(p-1)(4pq-3p-2)}{2}$.

Let $\Xi_{r,s} = \{uv \in E(G_1) : e(u) = r, e(v) = s\}$ be the set contain the edges with endpoints has the eccentricity r and s. From the above discussion, we have $|\Xi_{2,2}| = \frac{(p-1)(p+2q-4)}{2}$, $|\Xi_{2,3}| = (p - 1)(q - 1)(2p - 1)$. Mathematical formulation of above edge-based eccentric topological indices can be represent for graph G_1 in the following theorem.

Theorem 3.4.1. *For p, q be prime numbers. Let G_1 be the zero divisor graph containing commutative ring $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$, then first Zagreb eccentric index of G_1,*

$$M_1^*(G_1) = (p - 1)(10pq - 8p - q - 3)$$

the third Zagreb eccentric index

$$M_3^*(G_1) = 2(p-1)(6pq-5p-q-1)$$

the geometric-arithmetic eccentric index

$$GA_4(G_1) = (p-1)\left(\frac{p+2q-4}{2} + \frac{2\sqrt{6}}{5}(2p-1)(q-1)\right)$$

the atom-bond connectivity eccentric index

$$ABC_5(G_1) = \frac{1}{\sqrt{2}}|E(G_1)|$$

the fourth type of eccentric harmonic index

$$H_4(G_1) = \frac{p-1}{20}\left(16pq - 11p + 2q - 12\right).$$

Proof. By putting $|\Xi_{2,2}| = \frac{(p-1)(p+2q-4)}{2}$, $|\Xi_{2,3}| = (p-1)(q-1)(2p-1)$ in equations (2.26), (2.27), (2.28), (2.29) and (2.30), we obtain the required results. □

For verification purpose algorithmic results are compared by substituting some instances of the values of $a = p^2$ and $c = q$ in Theorem 3.4.1. It is observed that both results are same that proves the accuracy of algorithm. Some of the results are given in Table 3.2 for sake of computing fidelity and their use in future applications.

Figure 3.3 shows a pictorial representation of the results. Zero divisor graphs for $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$ with primes $p = a$, and $q = c$ are represented along the x-axis, and the topological indices are represented along the y-axis. The primes

Table 3.2: Algorithmic results of edge-based topological indices for zero divisor graph with $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$.

Case	$a = p^2$	$c = q$	Algorithmic Results				
			M_1	M_3	GA_4	ABC_5	Harmonic
1	2	3	38	44	7.879	5.657	3
2	3	5	232	272	47.192	33.941	20
3	5	7	1176	1392	235.636	169.706	98
4	7	11	4140	4920	824.241	593.970	342
5	11	13	13080	15600	2589.086	1866.762	1068
6	11	7	6540	7800	1294.543	933.381	534
7	13	5	6192	7392	1223.755	882.469	504
8	17	5	10816	12928	2133.329	1538.664	876
9	19	3	6804	8136	1341.088	967.322	550
10	23	3	10076	12056	1983.996	1431.184	814

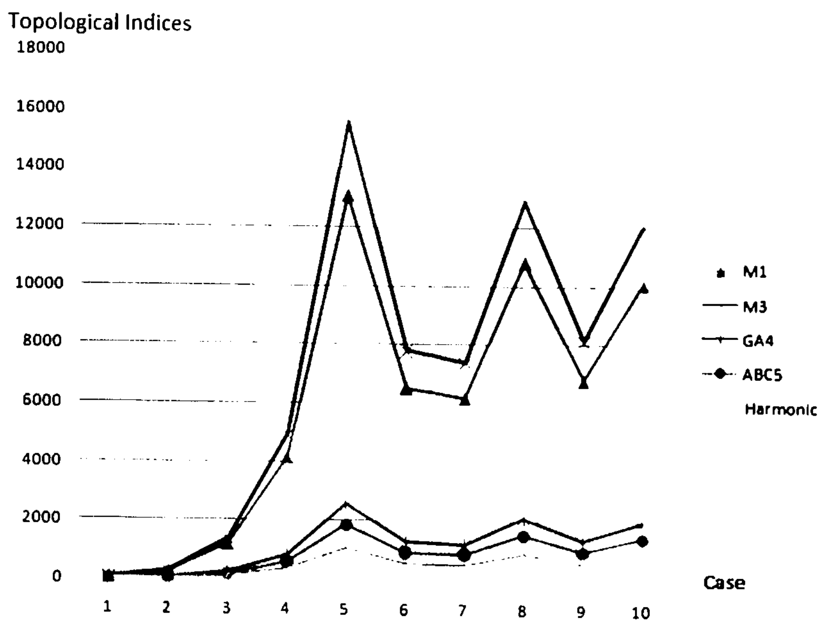


Figure 3.3: Plot of Table 3.2 results.

p and q are taken randomly. The values of topological indices were increasing in the initial five zero divisor graphs while increasing the value of p and q, the values were decreased at the sixth and seventh graphs, when p was increasing while q was decreasing, the values were increased again while increasing p and decreasing q. Thus, q has a stronger impact on topological indices. In all the graphs, M_3 has the largest value, the harmonic index has the smallest value, ABC_5 is greater than the harmonic index, GA_4 is greater than the ABC_5 index, and M_1 is greater than GA_4 index.

Case 2: $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$

For $a = p_1p_2$ and $b = q$, where p_1, p_2, q are prime numbers. Let G_2 be a zero divisor graph containing commutative ring $R = \mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$. We obtain $\mathsf{V}_t(G_2)$ with $t = p_1p_2 - 1, p_1q - 1, p_2q - 1, q - 1, p_1 - 1, p_2 - 1$ and $|\mathsf{V}_{p_1p_2-1}| = q - 1$, $|\mathsf{V}_{p_1q-1}| = p_2 - 1$, $|\mathsf{V}_{p_2q-1}| = p_1 - 1$, $|\mathsf{V}_{q-1}| = (p_1 - 1)(p_2 - 1)$, $|\mathsf{V}_{p_1-1}| = (p_2 - 1)(q - 1)$, $|\mathsf{V}_{p_2-1}| = (p_1 - 1)(q - 1)$. By hand shaking lemma $|E(G_2)| = 3p_1p_2q - 2p_1p_2 - 2p_1q - 2p_2q + p_1 + p_2 + q$. Let $\Xi_{r,s} = \{uv \in E(G_2) : e(u) = r, e(v) = s\}$ be the set contain the edges with endpoints has the eccentricity r and s. From the above discussion, we have $|\Xi_{2,2}| = p_1p_2 + p_1q + p_2q - 2p_1 - 2p_2 - 2q + 3$, $|\Xi_{2,3}| = 3p_1p_2q - 3p_1p_2 - 3p_1q - 3p_2q + 3p_1 + 3p_2 + 3q - 3$. Mathematical formulation of above edge-based eccentric topological indices can be represent for graph G_2 in the following theorem.

Theorem 3.4.2. *For $p_1 < p_2$ and q be prime numbers. Let G_2 be the zero divisor graph containing commutative ring $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$, then first Zagreb eccentric index is*

$$M_1^*(G_2) = 15p_1p_2q - 11\,(p_1p_2 + p_1q + p_2q) + 7\,(p_1 + p_2 + q) - 3$$

the third Zagreb eccentric index is

$$M_3^*(G_2) = 18p_1p_2q - 14\,(p_1p_2 + p_1q + p_2q) + 10\,(p_1 + p_2 + q) - 6$$

the geometric-arithmetic eccentric index is

$$\begin{aligned} GA_4(G_1) =& \frac{6\sqrt{6}}{5}\,(p_1p_2q - 1) + \left(1 - \frac{6\sqrt{6}}{5}\right)(p_1p_2 + p_1q + p_2q) \\ &+ \left(\frac{6\sqrt{6}}{5} - 2\right)(p_1 + p_2 + q) + 3. \end{aligned}$$

Table 3.3: Algorithmic results of edge-based topological indices for zero divisor graph with $\mathbb{Z}_{p_1 p_2} \times \mathbb{Z}_q$.

				Algorithmic Results				
Case	a	b	c	M_1	M_3	GA_4	ABC_5	Harmonic
1	2	3	5	176	200	37.515	26.870	16
2	3	5	5	608	704	126.060	50.912	54
3	5	7	5	1696	1984	346.181	248.902	147
4	5	11	7	4096	4816	829.453	596.798	350
5	7	11	7	6024	7104	1214.180	873.984	510
6	11	13	7	11808	13968	2368.359	1705.542	990
7	13	17	5	12736	15040	2561.450	1844.135	1073.6
8	17	19	5	18976	22432	3810.175	2743.574	1594
9	19	23	3	13784	16160	2803.995	2016.669	1188
10	23	29	2	11904	13752	2476.663	1777.666	1072

the atom-bond connectivity eccentric index is

$$ABC_5(G_2) = \frac{1}{\sqrt{2}}|E(G_2)|$$

the fourth type of eccentric harmonic index is

$$H_4(G_2) = \frac{6}{5}\left(p_1p_2q\right) - \frac{7}{10}\left(p_1p_2 + p_1q + p_2q\right) + \frac{1}{5}\left(p_1 + p_2 + q\right) + \frac{3}{10}.$$

Proof. By equating $|\Xi_{2,2}| = p_1p_2 + p_1q + p_2q - 2p_1 - 2p_2 - 2q + 3$, $|\Xi_{2,3}| = 3p_1p_2q - 3p_1p_2 - 3p_1q - 3p_2q + 3p_1 + 3p_2 + 3q - 3$ in equations (2.26), (2.27), (2.28), (2.29) and (2.30), we obtain the required results. □

For verification purpose algorithmic results are compared by substituting some instances of the values of $a = p_1, b = p_2$ and $c = q$ in Theorem 3.4.1. It is observed that both results are same that proves the accuracy of algorithm. Some of the results are given in Table 3.3 for sake of computing fidelity and their use in future applications.

Figure 3.4 shows a pictorial representation of the results. Zero divisor

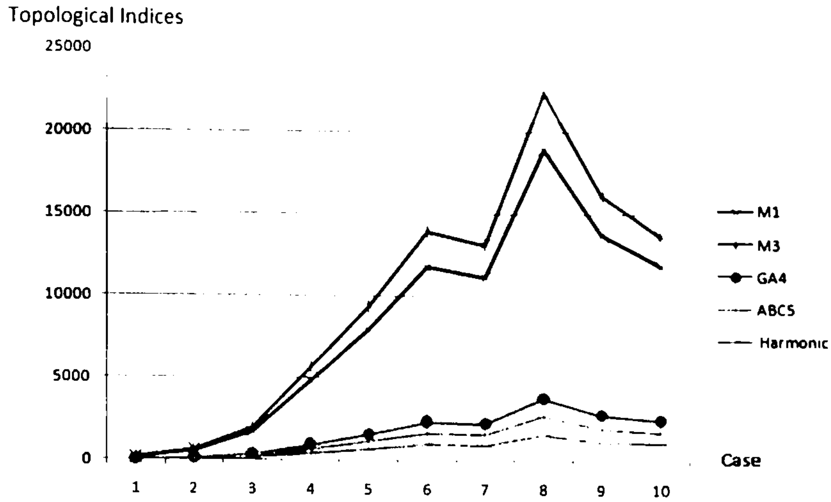


Figure 3.4: Plot of Table 3.3 results.

graphs for $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$ with primes $p_1 = a$, $p_2 = b$, and $q = c$ are represented along x-axis, and the topological indices are represented along the y-axis. The primes p_1, p_2 and q are taken randomly with condition $p_1 < p_2$. The values of topological indices were increasing in initial eight zero divisor graphs while increasing the value of q, at the ninth zero divisor graph, the value q decreased. as a result, the values of topological indices also decreased. Thus, q has a stronger impact on topological indices. In all the graphs, M_3 has the largest value, the harmonic index has the smallest value, ABC_5 is greater than the harmonic index, GA_4 is greater than the ABC_5 index, and M_1 is greater than GA_4 index.

CHAPTER 4

DEGREE BASED TOPOLOGICAL INDICES

In this chapter, degree based topological indices are computed for line graph of benzene ring embedded in the P-type-surface network, line graph by utilizing the system of subdivision of benzene ring embedded in the P-type-surface network, graph of conductive 2D MOD, line graph of conductive 2D MOD and line graph by utilizing the system of subdivision of conductive 2D MOD.

4.1 Degree Based Topological Indices

Degree based topological indices are computed from the degree of vertices in the graph. A standout amongst the most critical topological index is the outstanding stretching index presented by Randić [77] which is characterized as the whole of certain bond commitments ascertained from the vertex level of the hydrogen stifled atomic graphs. This index was discovered reasonable with the end goal of medication plan [77]. The numerical elements of Randić index incorporates its association with the standardized Laplacian framework [19]. Ghorbani and Azimi defined two new versions of Zagreb indices of a graph G in 2012 [50]. 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 in equations (2.13),(2.14),(2.15) and (2.16), respectively.

Urtula *et al.* [44] introduced an augmented Zagreb index see equation (2.11). Estrada, Torres, Rodriguez and Gutman [34] have introduced *atom-bond connectivity index* (ABC index) in equation (2.7). Ghorbani and Hosseinzadeh [49] obtained the updated version of ABC index termed as ABC_4 index that is shown in equation (2.8). Vukičević and Furtula [89] defined *geometric-arithmetic index* (GA index) as shown in equation (2.9) and Graovac, Ghorbani and Hosseinzadeh [53] introduced extended version of GA index termed as GA_5 index and shown in equation (2.10). Farahani, Ediz and Imran [42] introduced the Harmonic index in equation (2.5). In the section, we determine these indices for line and para-line graph of benzene ring and chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$.

4.2 Line graph and line graph of subdivision of benzene ring

The topological indices of benzene ring embedded in P-type-surface in 2D network are computed by Ahmad in [1]. Now onward, benzene ring embedded in P-type-surface in 2D network is denoted by G as shown in Figure 4.1, its line graph is denoted by $L(G)$ and line graph of subdivision of G is denoted by $L(S(G))$. The line graph of G is shown in Figure 4.2.

4.2.1 Topological Indices of Line Graph of Benzene Ring

In this section, we determine the topological indices of line graph of benzene ring embedded in P-type-surface in 2D network, namely Randic index, general sum-connectivity index, atom-bond connectivity index, geometric-arithmetic index, fourth version of atom-bond connectivity index and fifth version of geometric-arithmetic index.

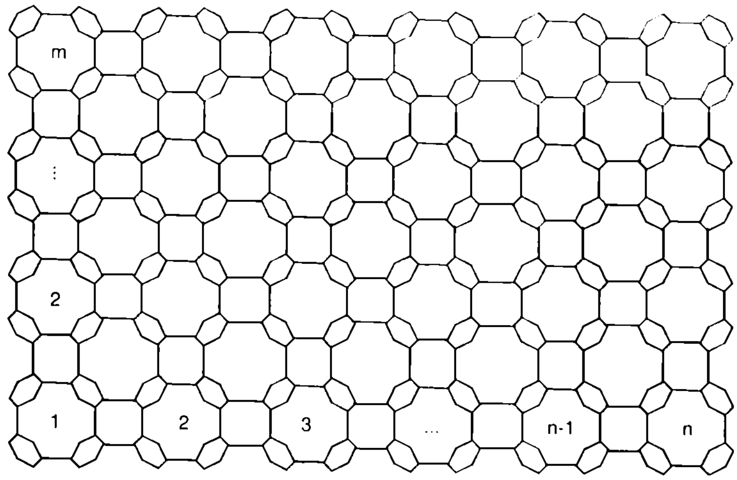


Figure 4.1: Benzene ring embedded in the P-type-surface network.

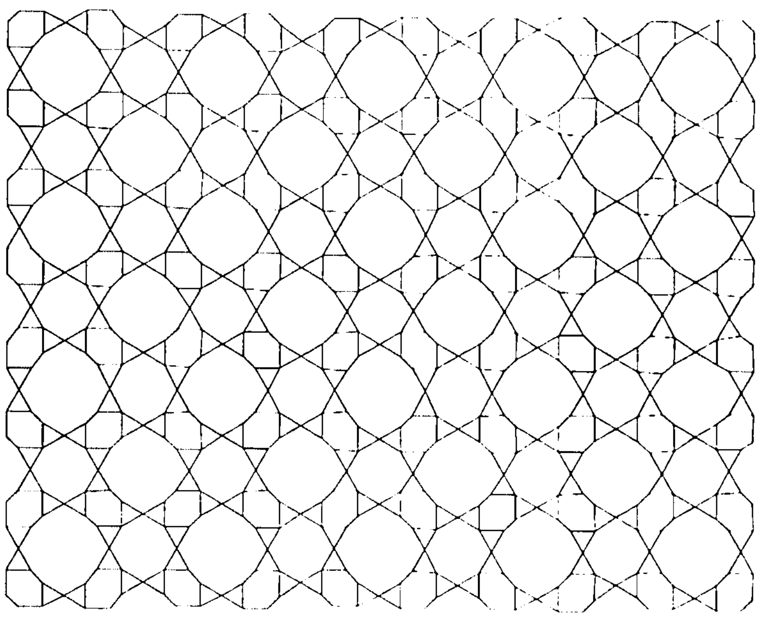


Figure 4.2: The line of G with $n = 5$ and $m = 4$.

The line graph of the benzene ring in the P-type surface is shown in Figure 4.2. For our convenience, we suppose that there are n number of benzene rings in any row and m number of benzene rings in any column. The total number of vertices in this graph are $32mn - 2m - 2n$, among which $4m + 4n$ vertices are of degree 2, $16mn$ vertices are of degree 3, and $16mn - 6m - 6n$ vertices are of degree 4 as represented in the vertex partition in Table 4.1.

Let $e_{u,v}$ denotes the number of edges connecting the vertices of degree d_u and d_v. The line graph of the benzene ring in the P-type surface contains

Table 4.1: The vertex partition of $L(G)$ based on degree of vertices.

Degree of vertex	Number of vertices
2	$4m + 4n$
3	$16mn$
4	$16mn - 6m - 6n$
Total	$32mn - 2m - 2n$

only $e_{2,2}$, $e_{2,3}$, $e_{3,3}$, $e_{3,4}$, and $e_{4,4}$ edges. These edges are mentioned in the edge partition in Table 4.2.

Table 4.2: The edge partition of $L(G)$ based on degree of end vertices of each edge.

(d_{x_1}, d_{x_2}), where $x_1x_2 \in E(G)$	Number of edges
$(2, 2)$	4
$(2, 3)$	$8m + 8n - 8$
$(3, 3)$	$8mn + 4$
$(3, 4)$	$32mn - 8m - 8n$
$(4, 4)$	$16mn - 8m - 8n$
Total	$56mn - 8m - 8n$

Theorem 4.2.1. *Let $L(G)$ be a line graph of G and α is a real number, then*

(1) $M_\alpha(L(G)) = (m+n)\, 2^{\alpha+2} + (8\, mn - 3\, m - 3\, n)\, 2^{2\alpha+1} + (16\, mn)\, 3^\alpha,$

(2) $R_\alpha(L(G)) = 2^{2\alpha+2} + 2^{\alpha+3}\, (m+n-1)\, 3^\alpha + (2mn - m - n)\, 2^{4\alpha+3}$

$+\, 2^{2\alpha+3}\, (4\, mn - m - n)\, 3^\alpha + 4\, (2\, mn + 1)\, 3^{2\alpha},$

(3) $\chi_\alpha(L(G)) = 2^{2\alpha+2} + (8\, m + 8\, n - 8)\, 5^\alpha + (8\, mn + 4)\, 6^\alpha$

$+\, (32\, mn - 8\, m - 8\, n)\, 7^\alpha + (16\, mn - 8\, m - 8\, n)\, 8^\alpha.$

Proof. The vertex partition with respect to the degree of vertices of $L(G)$ is calculated in Table 4.1. The edge partition with respect the degree of end vertices of $L(G)$ is calculated in Table 4.2. By putting the values calculated in Table 4.1 and Table 4.2 in equations 2.2, 2.3, and 2.6, and by simplifying them with the help of Maple, we determine the general Randic index, general sum-connectivity index and general Zagreb index as follows:

$$\begin{aligned} R_\alpha(L(G)) &= \sum_{x_1x_2\in E(L(G))} (d_{x_1}d_{x_2})^\alpha \\ &= e_{2,2}(2\times 2)^\alpha + e_{2,3}(2\times 3)^\alpha + e_{3,3}(3\times 3)^\alpha 13 + e_{3,4}(3\times 4)^\alpha \\ &\quad + e_{4,4}(4\times 4)^\alpha \\ &= (4)4^\alpha + (8m+8n-8)6^\alpha + (8mn+4)9^\alpha + \\ &\quad (32mn-8m-8n)12^\alpha + (32mn-8m-8n)16^\alpha \\ &= 2^{2\alpha+2} + 2^{\alpha+3}(m+n-1)\,3^\alpha + (2mn-m-n)\,2^{4\alpha+3} + \\ &\quad 2^{2\alpha+3}(4mn-m-n)\,3^\alpha + 4\,(2mn+1)\,3^{2\alpha}. \end{aligned}$$

$$\begin{aligned} \chi_\alpha(L(G)) &= \sum_{x_1x_2\in E(L(G))} (d_{x_1}+d_{x_2})^\alpha \\ &= e_{2,2}(2+2)^\alpha + e_{2,3}(2+3)^\alpha + e_{3,3}(3+3)^\alpha + e_{3,4}(3+4)^\alpha + e_{4,4}(4+4)^\alpha \\ &= (4)4^\alpha + (8m+8n-8)5^\alpha + (8mn+4)6^\alpha + (32mn-8m-8n)7^\alpha + \\ &\quad (32mn-8m-8n)8^\alpha \\ &= 2^{2\alpha+2} + (8m+8n-8)\,5^\alpha + (8mn+4)\,6^\alpha + (32mn-8m-8n)\,7^\alpha + \\ &\quad (16mn-8m-8n)\,8^\alpha. \end{aligned}$$

$$M_\alpha(L(G)) = (m+n)\,2^{\alpha+2} + (8mn-3m-3n)\,2^{2\alpha+1} + (16mn)\,3^\alpha.$$

This completes the proof. □

Theorem 4.2.2. *The ABC index and GA index for $L(G)$ is*

(1) $ABC(L(G)) = 2\sqrt{2} + \frac{1}{2}(8m + 8n - 8)\sqrt{2} + \frac{16}{3}mn + \frac{8}{3} + \frac{1}{6}(32mn - 8m - 8n)\sqrt{15} + \frac{1}{4}(16mn - 8m - 8n)\sqrt{6}.$

(2) $GA(L(G)) = 8 + \frac{2}{5}(8m + 8n - 8)\sqrt{6} + 24mn + \frac{4}{7}(32mn - 8m - 8n)\sqrt{3} - 8m - 8n.$

Proof. Let $e_{i,j}$ denotes the number of edges in the edge partition with degree of end vertices is i and j. By putting the values of edge partition of $L(G)$ calculated in Table 4.2 in equations (2.7) and (2.9), we determine the ABC index and GA index as:

$$\begin{aligned} ABC(L(G)) &= \sum_{x_1x_2 \in E(L(G))} \sqrt{\frac{d_{x_1}+d_{x_2}-2}{d_{x_1}\times d_{x_2}}} \\ &= e_{2,2}\sqrt{\frac{2+2-2}{2\times 2}} + e_{2,3}\sqrt{\frac{2+3-2}{2\times 3}} + e_{3,3}\sqrt{\frac{3+3-2}{3\times 3}} + e_{3,4}\sqrt{\frac{3+4-2}{3\times 4}} + \\ &\quad e_{4,4}\sqrt{\frac{4+4-2}{4\times 4}}. \end{aligned}$$

After simplification, we obtain

$$\begin{aligned} ABC(L(G)) &= 2\sqrt{2} + \frac{1}{2}(8m + 8n - 8)\sqrt{2} + \frac{16}{3}mn + \frac{8}{3} + \\ &\quad \frac{1}{6}(32mn - 8m - 8n)\sqrt{15} + \frac{1}{4}(16mn - 8m - 8n)\sqrt{6}. \end{aligned}$$

$$\begin{aligned}
GA(L(G)) &= \sum_{uv\in E(L(G))} \frac{2\sqrt{d(u)\times d(v)}}{d(u)+d(v)} \\
&= e_{2,2}\frac{2\sqrt{2\times 2}}{2+2} + e_{2,3}\frac{2\sqrt{2\times 3}}{2+3} + e_{3,3}\frac{2\sqrt{3\times 3}}{3+3} + e_{3,4}\frac{2\sqrt{3\times 4}}{3+4} + \\
&\quad e_{4,4}\frac{2\sqrt{4\times 4}}{4+4} \\
&= (4)\frac{2\times 2}{4} + (8m+8n-8)\frac{2\sqrt{6}}{5} + (8mn+4)\frac{2\times 3}{6} + \\
&\quad (32mn-8m-8n)\frac{2\sqrt{12}}{7} + (16mn-8m-8n)\frac{2\times 4}{8}.
\end{aligned}$$

After simplification, we obtain

$$\begin{aligned}
GA(L(G)) &= 8 + \frac{2}{5}(8m+8n-8)\sqrt{6} + 24mn + \\
&\quad \frac{4}{7}(32mn-8m-8n)\sqrt{3} - 8m - 8n.
\end{aligned}$$

This completes the proof. □

In the following theorems, we present the fourth atom-bond connectivity index (ABC_4) and the fifth geometric-arithmetic index (GA_5). Table 4.3 represents the edge partitions based on degree sum of neighbor vertices of end vertices of each edge in $L(G)$. We use this partition of edges to calculate ABC_4 and GA_5 indices. The edge set $E(L(G))$ divided into thirteen edge partitions based on degree of end vertices. The edge partition $E_{x_1,x_2}(L(G))$ contains m_{x_1,x_2} edges x_1x_2, where $S(x_1)=x_1$, $S(x_2)=x_2$ and $m_{x_1,x_2}=|E_{x_1,x_2}(L(G))|$.

Theorem 4.2.3. *The ABC_4 index and GA_5 index for $L(G)$ is*

(1) $ABC_4(L(G)) = \frac{14}{5}\sqrt{2} + \frac{16}{15}\sqrt{15} + \frac{1}{18}(4m+4n-8)\sqrt{78} + \frac{1}{30}$
$(4m+4n-8)\sqrt{210} + \frac{1}{30}(4m+4n)\sqrt{170} + \frac{1}{18}(4m+4n)\sqrt{57} + \frac{1}{110}$

Table 4.3: The edge partition of graph G based on degree sum of neighbor vertices of end vertices of each edge.

(S_{x_1}, S_{x_2}), where $x_1x_2 \in E(G)$	Number of edges
$(5,5)$	4
$(5,9)$	8
$(6,9)$	$4m+4n-8$
$(6,10)$	$4m+4n-8$
$(9,10)$	$4m+4n$
$(9,12)$	$4m+4n$
$(10,10)$	4
$(10,11)$	$4m+4n-8$
$(10,12)$	$4m+4n$
$(10,14)$	$8m+8n-16$
$(11,11)$	$8mn-8m-8n+8$
$(11,14)$	$32mn-24m-24n+16$
$(14,14)$	$16mn-8m-8n$
Total	$56mn-8m-8n$

$(4m+4n-8)\sqrt{2090} + \frac{1}{6}(4m+4n)\sqrt{6} + \frac{1}{70}(8m+8n-16)\sqrt{770} + \frac{2}{11}(8mn-8m-8n+8)\sqrt{5} + \frac{1}{154}(32mn-24m-24n+16)\sqrt{3542} + \frac{1}{14}(16mn-8m-8n)\sqrt{26}.$

(2) $GA_5(L(G)) = 16 + \frac{24}{7}\sqrt{5} + \frac{2}{5}(4m+4n-8)\sqrt{6} + \frac{1}{4}(4m+4n-8)\sqrt{15} + \frac{6}{19}(4m+4n)\sqrt{10} + \frac{4}{7}(4m+4n)\sqrt{3} + \frac{2}{21}(4m+4n-8)\sqrt{110} + \frac{2}{11}(4m+4n)\sqrt{30} + \frac{1}{6}(8m+8n-16)\sqrt{35} + 24mn - 16m - 16n + \frac{2}{25}(32mn-24m-24n+16)\sqrt{154}.$

Proof. Let $m_{i,j}$ denotes the number of edges of $L(G)$ with $i = S_{x_1}$ and $j = S_{x_2}$. It is easy to see that the summation of degree of edge endpoints of given graph has thirteen edge types $m_{5,5}$, $m_{5,9}$, $m_{6,9}$, $m_{6,10}$, $m_{9,10}$, $m_{9,12}$, $m_{10,10}$, $m_{10,11}$, $m_{10,12}$, $m_{10,14}$, $m_{11,11}$, $m_{11,14}$ and $m_{14,14}$ that are calculated in Table 4.3. By using these values in equations (2.8) and (2.10), we get the following:

$$ABC_4(L(G)) = \sum_{x_1x_2 \in E(L(G))} \sqrt{\frac{S_{x_1}+S_{x_2}-2}{S_{x_1} \times S_{x_2}}}$$

$$= m_{5,5}\sqrt{\frac{5+5-2}{5\times5}} + m_{5,9}\sqrt{\frac{5+9-2}{5\times9}} + m_{6,9}\sqrt{\frac{6+9-2}{6\times9}} + m_{6,10}\sqrt{\frac{6+10-2}{6\times10}} + m_{9,10}\sqrt{\frac{9+10-2}{9\times10}} + m_{9,12}\sqrt{\frac{9+12-2}{9\times12}} + m_{10,10}\sqrt{\frac{10+10-2}{10\times10}} + m_{10,11}\sqrt{\frac{10+11-2}{10\times11}} + m_{10,12}\sqrt{\frac{10+12-2}{10\times12}} + m_{10,14}\sqrt{\frac{10+14-2}{10\times14}} + m_{11,11}\sqrt{\frac{11+11-2}{11\times11}} + m_{11,14}\sqrt{\frac{11+14-2}{11\times14}} + m_{14,14}\sqrt{\frac{14+14-2}{14\times14}}$$

$$= 4\sqrt{\tfrac{8}{25}} + 8\sqrt{\tfrac{12}{45}} + (4m+4n-8)\sqrt{\tfrac{13}{54}} + (4m+4n-8)\sqrt{\tfrac{14}{60}} + (4m+4n)\sqrt{\tfrac{17}{90}} + (4m+4n)\sqrt{\tfrac{19}{108}} + 4\sqrt{\tfrac{18}{100}} + (4m+4n-8)\sqrt{\tfrac{19}{110}} + (4m+4n)\sqrt{\tfrac{20}{120}} + (8m+8n-16)\sqrt{\tfrac{22}{140}} + (8mn-8m-8n+8)\sqrt{\tfrac{20}{121}} + (32mn-24m-24n+16)\sqrt{\tfrac{23}{154}} + (16mn-8m-8n)\sqrt{\tfrac{26}{196}}.$$

and

$$GA_5(L(G)) = \sum_{x_1x_2\in E(L(G))} \frac{2\sqrt{S_{x_1}\times S_{x_2}}}{S_{x_1}+S_{x_2}}$$

$$= m_{5,5}\frac{2\sqrt{5\times5}}{5+5} + m_{5,9}\frac{2\sqrt{5\times9}}{5+9} + m_{6,9}\frac{2\sqrt{6\times9}}{6+9} + m_{6,10}\frac{2\sqrt{6\times10}}{6+10} + m_{9,10}\frac{2\sqrt{9\times10}}{9+10} + m_{9,12}\frac{2\sqrt{9\times12}}{9+12} + m_{10,10}\frac{2\sqrt{10\times10}}{10+10} + m_{10,11}\frac{2\sqrt{10\times11}}{10+11} + m_{10,12}\frac{2\sqrt{10\times12}}{10+12} + m_{10,14}\frac{2\sqrt{10\times14}}{10+14} + m_{11,11}\frac{2\sqrt{11\times11}}{11+11} + m_{11,14}\frac{2\sqrt{11\times14}}{11+14} + m_{14,14}\frac{2\sqrt{14\times14}}{14+14}$$

$$= 4\tfrac{2\sqrt{25}}{10} + 8\tfrac{2\sqrt{45}}{14} + (4m+4n-8)\tfrac{2\sqrt{54}}{15} + (4m+4n-8)\tfrac{2\sqrt{60}}{16} + (4m+4n)\tfrac{2\sqrt{90}}{19} + (4m+4n)\tfrac{2\sqrt{108}}{21} + 4\tfrac{2\sqrt{100}}{20} + (4m+4n-8)\tfrac{2\sqrt{110}}{21} + (4m+4n)\tfrac{2\sqrt{120}}{22} + (8m+8n-16)\tfrac{2\sqrt{140}}{24} + (8mn-8m-8n+8)\tfrac{2\sqrt{121}}{22} + (32mn-24m-24n+16)\tfrac{2\sqrt{154}}{25} + (16mn-8m-8n)\tfrac{2\sqrt{196}}{28}.$$

After simplification, we obtain the desired results. □

4.2.2 Topological Indices of line graph of subdivision of Benzene Ring

The line graph of subdivision of G is shown in Figure 4.3. In this section, we determine the topological indices of line graph of subdivision of benzene ring, namely namely generalized Randic, general Zagreb, general sum-connectivity, ABC, GA, ABC_4 and GA_5 indices.

Theorem 4.2.4. *Let $L(S(G))$ be a line graph of subdivision of G, then*

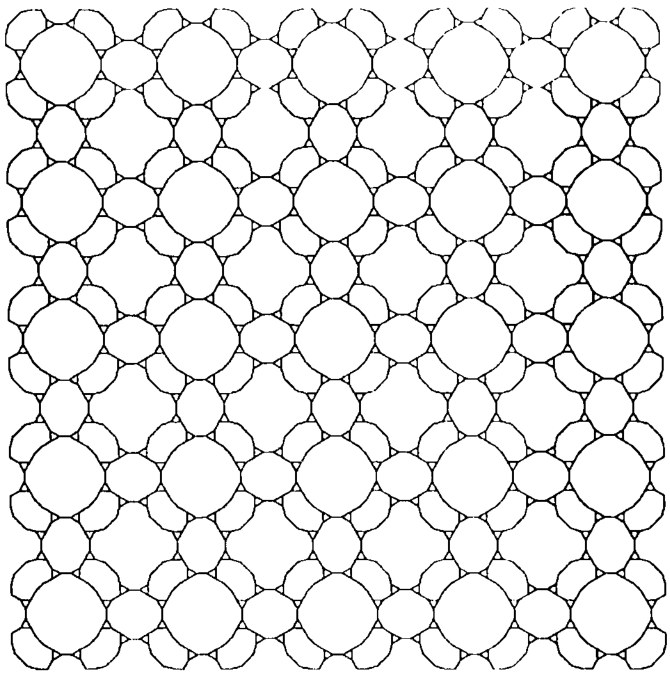


Figure 4.3: The line graph of subdivision of G with $n = 5$ and $m = 5$.

Table 4.4: The vertex partition of $L(S(G))$ based on degree of vertices.

Degree of vertex	Number of vertices
2	$16mn + 8m + 8n$
3	$48mn - 12m - 12n$
Total	$64mn - 4m - 4n$

Table 4.5: The edge partition of $L(S(G))$ based on degree of end vertices of each edge.

(d_{x_1}, d_{x_2}), where $x_1x_2 \in E(L(S(G)))$	Number of edges
$(2,2)$	$8mn + 8m + 8n$
$(2,3)$	$16mn$
$(3,3)$	$64mn - 18m - 18n$
Total	$88mn - 10m - 10n$

(1) $M_\alpha(L(S(G))) = (2mn + m + n)2^{\alpha+3} + 4(4mn - m - n)3^{\alpha+1}$,

(2) $R_\alpha(L(S(G))) = (mn + m + n)2^{2\alpha+3} + (64mn - 18m - 18n)3^{2\alpha} + (16mn)6^{\alpha}$,

(3) $\chi_\alpha(L(S(G))) = (mn + m + n)2^{2\alpha+3} + (16mn)5^{\alpha} + (64mn - 18m - 18n)6^{\alpha}$,

where α is a real number.

Proof. The vertex partition with respect to the degree of vertices of $L(S(G))$ is calculated in Table 4.4. By using these values in the formula of first general Zagreb index defined in equation (2.6), we obtain the result.

Let e_{x_1,x_2} denotes the number of edges connecting the vertices of degree d_{x_1} and d_{x_2}. The edge partition with respect the degree of end vertices of $L(S(G))$ is calculated in Table 4.5. By using these values in the formula of general Randić index defined in equation (2.2) and in the formula of general sum-connectivity index defined in equation (2.3), we obtain the following results:

$$R_\alpha(L(S(G))) = \sum_{x_1x_2\in E(L(S(G))} (d_{x_1}d_{x_2})^\alpha$$
$$= e_{2,2}\,(2\times 2)^\alpha + e_{2,3}\,(2\times 3)^\alpha + e_{3,3}\,(3\times 3)^\alpha$$
$$= (8mn+8m+8n)4^\alpha + (16mn)6^\alpha + (64mn-18m-18n)9^\alpha$$
$$= (mn+m+n)2^{2\alpha+3} + (64mn-18m-18n)3^{2\alpha} + (16mn)6^\alpha.$$

$$\chi_\alpha(L(S(G))) = \sum_{x_1x_2\in E(L(S(G)))} (d_{x_1}+d_{x_2})^\alpha$$
$$= e_{2,2}\,(2+2)^\alpha + e_{2,3}\,(2+3)^\alpha + e_{3,3}\,(3+3)^\alpha$$
$$= (8mn+8m+8n)4^\alpha + (16mn)5^\alpha + (64mn-18m-18n)6^\alpha$$
$$= (mn+m+n)2^{2\alpha+3} + (16mn)5^\alpha + (64mn-18m-18n)6^\alpha.$$

This completes the proof. □

Theorem 4.2.5. *Let $L(S(G))$ be the line graph of the subdivision graph of G. Then its ABC index and GA index for $L(S(G))$ is:*

(1) $ABC(L(S(G))) = \left(12\sqrt{2}+\frac{128}{3}\right)mn + \frac{1}{2}(8m+8n)\sqrt{2} - 12n - 12m.$

(2) $GA(L(S(G))) = \left(72+\frac{32}{5}\sqrt{6}\right)mn - 10m - 10n.$

Proof. By using the values of edge partition calculated from Table 4.5 of graph $L(S(G))$ in the formula of ABC index and GA index. After simplification, we obtain the required results. □

Table 4.6: The edge partition of graph $L(S(G))$ based on degree sum of neighbor vertices of end vertices of each edge.

(S_{x_1}, S_{x_2}), where $x_1x_2 \in E(L(S(G)))$	Number of edges
$(4,4)$	$4m + 4n + 4$
$(4,5)$	$8m + 8n - 8$
$(5,5)$	$8mn - 4m - 4n + 4$
$(5,8)$	$16mn$
$(8,8)$	$4m + 4n$
$(8,9)$	$32mn - 8m - 8n$
$(9,9)$	$32mn - 14m - 14n$
Total	$88mn - 10m - 10n$

Let $m_{i,j}$ denotes the number of edges of $L(S(G))$ with $i = S_{x_1}$ and $j = S_{x_2}$. It is easy to see that the summation of degree of edge endpoints of given graph has seven edge types $m_{4,4}$, $m_{4,5}$, $m_{5,5}$, $m_{5,8}$, $m_{8,8}$, $m_{8,9}$, and $m_{9,9}$ that are calculated in Table 4.6.

In the next two theorems, we calculate the fourth atom-bond connectivity index ABC_4 and the fifth geometric-arithmetic index GA_5. There are seven types of edges on degree based sum of neighbors vertices of each edge in $L(S(G))$. We use this partition of edges to calculate ABC_4 and GA_5 indices. Table 4.6 gives such types of edges of $L(S(G))$. The edge set $E(L(S(G)))$ divided into seven edge partitions based on degree of end vertices. The edge partition $E_{x_1,x_2}(L(S(G)))$ contains m_{x_1,x_2} edges x_1x_2, where $S_{x_1} = x_1$, $S_{x_2} = x_2$ and $m_{x_1,x_2} = |E_{x_1,x_2}(L(S(G)))|$.

Theorem 4.2.6. *The fourth atom-bound connectivity index ABC_4 of $L(S(G))$ is* *given by*

$$
\begin{aligned}
ABC_4(L(S(G))) &= \left(\frac{16}{5}\sqrt{2}+\frac{4}{5}\sqrt{110}+\frac{8}{3}\sqrt{30}+\frac{128}{9}\right)mn+ \\
&\frac{1}{4}(4m+4n+4)\sqrt{6}+\frac{1}{10}(8m+8n-8)\sqrt{35}+ \\
&\frac{2}{5}(-4m-4n+4)\sqrt{2}+\frac{1}{8}(4m+4n)\sqrt{14}+ \\
&\frac{1}{12}(-8m-8n)\sqrt{30}-\frac{56}{9}m-\frac{56}{9}n.
\end{aligned}
$$

Proof. By the definition of ABC_4 index and using the values from Table 4.6, we obtain

$$
\begin{aligned}
ABC_4(L(S(G))) &= \sum_{x_1x_2\in E(L(S(G)))}\sqrt{\tfrac{S_{x_1}+S_{x_2}-2}{S_{x_1}\times S_{x_2}}} \\
&= (4m+4n+4)\sqrt{\tfrac{4+4-2}{4\times4}}+(8m+8n-8)\sqrt{\tfrac{4+5-2}{4\times5}}+ \\
&(8mn-4m-4n+4)\sqrt{\tfrac{5+5-2}{5\times5}}+(16mn)\sqrt{\tfrac{5+8-2}{5\times8}}+ \\
&(4m+4n)+\sqrt{\tfrac{8+8-2}{8\times8}}(32mn-8m-8n)\sqrt{\tfrac{8+9-2}{8\times9}}+ \\
&(32mn-14m-14n)\sqrt{\tfrac{9+9-2}{9\times9}}.
\end{aligned}
$$

After simplification, we obtain the desired result. □

Theorem 4.2.7. *The fifth geometric-arithmetic index GA_5 of $L(S(G))$ is given by*

$$
\begin{aligned}
GA_5(L(S(G))) &= \left(40+\frac{64}{13}\sqrt{10}+\frac{384}{17}\sqrt{2}\right)mn-10m-10n+ \\
&8+\frac{4}{9}(8m+8n-8)\sqrt{5}+\frac{12}{17}(-8m-8n)\sqrt{2}.
\end{aligned}
$$

Proof. By the definition of GA_5 index and using the values from Table 4.6, we obtain

$$
\begin{aligned}
GA_5(L(S(G))) &= \sum_{x_1x_2 \in E(L(S(G)))} \frac{2\sqrt{S_{x_1} \times S_{x_2}}}{S_{x_1} + S_{x_2}} \\
&=(4m+4n+4)\frac{2\sqrt{4\times 4}}{4+4} + (8m+8n-8)\frac{2\sqrt{4\times 5}}{4+5} + \\
&(8mn-4m-4n+4)\frac{2\sqrt{5\times 5}}{5+5} + (16mn)\frac{2\sqrt{5\times 8}}{5+8} + \\
&(4m+4n)\frac{2\sqrt{8\times 8}}{8+8} + (32mn-8m-8n)\frac{2\sqrt{8\times 9}}{8+.9} + \\
&(32mn-14m-14n)\frac{2\sqrt{9\times 9}}{9+9} \\
&= \left(40 + \frac{64}{13}\sqrt{10} + \frac{384}{17}\sqrt{2}\right) mn - 10m - 10n + 8 + \frac{4}{9} \\
&(8m+8n-8)\sqrt{5} + \frac{12}{17}(-8m-8n)\sqrt{2}.
\end{aligned}
$$

This completes the proof. □

4.3 Chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$

$Cu_3(HITP)_2(HITP = 2,3,6,7,10,11-$hexaiminotriphenylene) is an incipient electrically conductive 2D MOF.

The graph of chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$ is shown in Figure 4.4. These graphs consists of a main hexagons and minor hexagons. For our convenient, we suppose that there are m number of main hexagons in any row and n number of main hexagons in any column. The number of vertices in this graph are $72mn + 22n + 2m$ among which $30mn + 14n + 4m$ vertices are of degree 2 and $42mn + 8n - 2m$ vertices are of degree 3, by Table 4.7.

Let $\delta(G)$ and $\Delta(G)$ be the minimum and maximum degree of G,

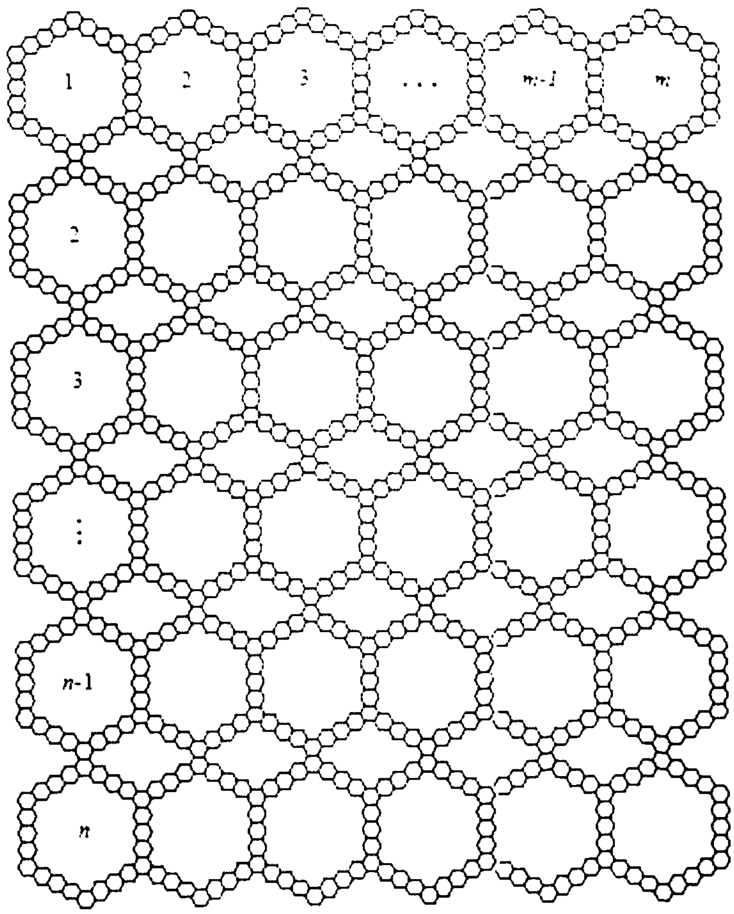


Figure 4.4: The graph of chemical structures of the conductive 2D MOFs.

respectively. The edge set $E(G)$ can be divided into several partitions: for any i and j, $\delta(G) \leq i, j \leq \Delta(G)$, let $E_{ij} = \{e = x_1x_2 \in E(G) : d_{x_1} = i, d_{x_2} = j\}$, $e_{i,j} = |E_{ij}|$, and $V_i = \{x_1 \in V(G) : d_{x_1} = i\}$, $n_i = |V_i|$.

Table 4.7: The vertex partition of graph G based on degree of vertices.

Degree of vertex	Number of vertices
2	$30mn + 14n + 4m$
3	$42mn + 8n - 2m$
Total	$72mn + 22n + 2m$

Table 4.8: The edge partition of graph G based on degree of end vertices of each edge.

(d_{x_1}, d_{x_2}), where $x_1x_2 \in E(G)$	Number of edges
$(2,2)$	$4n + 2m$
$(2,3)$	$60mn + 20n + 4m$
$(3,3)$	$33mn + 2n - 5m$
Total	$93mn + 26n + m$

Theorem 4.3.1. *Let G be a chemical structures of the conductive 2D MOFs*

$Cu_3(HITP)_2[m,n]$ with m is the number of main hexagons in any row and n is the number of main hexagons in any column. Then

1. $M_\alpha(G) = (15mn + 7n + 2m).2^{\alpha+1} + 2(21mn + 4n - m).3^\alpha$

2. $R_\alpha(G) = (2n + m).2^{2\alpha+1} + (33mn + 2n - 5m).3^{2\alpha} + 4(15mn + 5n + m).6^\alpha$

3. $\chi_\alpha(G) = (2n + m).2^{2\alpha+1} + 4(15mn + 5n + m).5^\alpha + (33mn + 2n - 5m).6^\alpha$.

   where α is a real number.

Proof. The graph of the chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$ is shown in Figure 4.4. Let e_{x_1,x_2} denotes the number of edges connecting the vertices of degree d_{x_1} and d_{x_2}. In this graph G there are total number of vertices are $72mn + 22n + 2m$. The number of vertices of degree two and three are $30mn + 14n + 4m$ and $42mn + 8n - 2m$, respectively, as shown in vertex partition in Table 4.7. By using these values in the formula of first general Zagreb index, we obtain the desired result.

The total number of edges of chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$ are $93mn + 26n + m$. The edge partition based on the degree of the end vertices of each edge as shown in Table 4.8. Since, the formula of general Randić index is

$$R_\alpha(G) = \sum_{x_1x_2 \in E(G)} (d_{x_1} d_{x_2})^\alpha,$$

this implies that

$R_\alpha(G) = e_{2,2}\,(2 \times 2)^\alpha + e_{2,3}\,(2 \times 3)^\alpha + e_{3,3}\,(3 \times 3)^\alpha$

$$= (4n + 2m).2^{2\alpha} + (60mn + 20n + 4m).6^{\alpha} + (33mn + 2n - 5m).3^{2\alpha}$$

$$= (2n + m).2^{2\alpha+1} + (33mn + 2n - 5m).3^{2\alpha} + 4(15mn + 5n + m).6^{\alpha}.$$

The formula of general sum-connectivity index is

$$\chi_\alpha(G) = \sum_{x_1x_2 \in E(G)} (d_{x_1} + d_{x_2})^{\alpha},$$

this implies that

$$\chi_\alpha(G) = e_{2,2}\,(2+2)^\alpha + e_{2,3}\,(2+3)^\alpha + e_{3,3}\,(3+3)^\alpha$$

$$= (4n + 2m).2^{2\alpha} + (60mn + 20n + 4m).5^{\alpha} + (33mn + 2n - 5m).6^{\alpha}$$

$$= (2n + m).2^{2\alpha+1} + 4(15mn + 5n + m).5^{\alpha} + (33mn + 2n - 5m).6^{\alpha}.$$

This completes the proof. □

Theorem 4.3.2. *The atom-bound connectivity index ABC of the chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$ is given by*

$$ABC(G) = (30\sqrt{2} + 22)mn + (2\sqrt{2} + 10\sqrt{2} + \frac{4}{3})n + (\sqrt{2} + 2\sqrt{2} - \frac{10}{3})m.$$

Proof. Consider the graph of the chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$. Let e_{x_1,x_2} denotes the number of edges connecting the vertices of degree d_{x_1} and d_{x_2}. Two-dimensional structure of the given graph contains only $e_{2,2}, e_{2,3}$ and $e_{3,3}$ edges. The number of $e_{2,2}, e_{2,3}$ and $e_{3,3}$ edges are mentioned in Table 4.8. Since, the atom-bond connectivity index is defined as

$$ABC(G) = \sum_{x_1x_2 \in E(G)} \sqrt{\frac{d_{x_1} + d_{x_2} - 2}{d_{x_1} \times d_{x_2}}},$$

this implies that

$$ABC(G) = e_{2,2}\sqrt{\frac{2+2-2}{2\times 2}} + e_{2,3}\sqrt{\frac{2+3-2}{2\times 3}} + e_{3,3}\sqrt{\frac{3+3-2}{3\times 3}}.$$

By using Table 4.8, we obtain

$$\begin{aligned} ABC(G) &= (4n+2m)\sqrt{\frac{2+2-2}{2\times 2}} + (60mn+20n+4m)\sqrt{\frac{2+3-2}{2\times 3}} + \\ & (33mn+2n-5m)\sqrt{\frac{3+3-2}{3\times 3}}. \end{aligned}$$

After simplification, we obtain the desired result. □

Theorem 4.3.3. *The geometric-arithmetic index GA of the chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$ is given by*

$$GA(G) = (33+24\sqrt{6})mn + (6+8\sqrt{6})n + (\frac{8\sqrt{6}}{5} - 3)m.$$

Proof. The number of $e_{2,2}, e_{2,3}$ and $e_{3,3}$ edges are mentioned in Table 4.8. Since the geometric-arithmetic index is defined as

$$GA(G) = \sum_{x_1x_2\in E(G)} \frac{2\sqrt{d_{x_1}\times d_{x_2}}}{d_{x_1}+d_{x_2}},$$

this implies that

$$GA(G) = e_{2,2}\frac{2\sqrt{2\times 2}}{2+2} + e_{2,3}\frac{2\sqrt{2\times 3}}{2+3} + e_{3,3}\frac{2\sqrt{3\times 3}}{3+3}.$$

By using Table 4.8, we obtain

$$GA(G) = (4n + 2m)\frac{2 \times 2}{4} + (60mn + 20n + 4m)\frac{2\sqrt{6}}{5} +$$
$$(33mn + 2n - 5m)\frac{2 \times 3}{6}.$$

After simplification, we obtain the desired result. □

In the next two theorems, we calculate the fourth atom-bond connectivity index ABC_4 and the fifth geometric-arithmetic index GA_5. There are nine types of edges on degree based sum of neighbors vertices of each edge in the chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$. We use this partition of edges to calculate ABC_4 and GA_5 indices. Table 4.9 gives such types of edges of the chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$.

Table 4.9: The edge partition of graph G based on degree sum of neighbor vertices of end vertices of each edge.

(S_{x_1}, S_{x_2}), where $x_1x_2 \in E(G)$	Number of edges
$(5,5)$	$4n + 2m$
$(5,7)$	$8n + 4m$
$(6,7)$	$40mn + 16n + 4m$
$(6,8)$	$20mn - 4n - 4m$
$(7,7)$	$10mn + 2n$
$(7,8)$	$8n + 4m$
$(8,8)$	$18mn - 8n - 4m$
$(8,9)$	$4mn - 4m$
$(9,9)$	$mn - m$
Total	$93mn + 26n + m$

Theorem 4.3.4. *The fourth atom-bound connectivity index ABC_4 of the*

chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$ is given by

$$\begin{aligned}ABC_4(G) &= \left(\frac{20}{21}\sqrt{462}+\frac{94}{9}+\frac{9}{4}\sqrt{14}+\frac{20}{7}\sqrt{3}+\frac{1}{3}\sqrt{30}\right)mn+\\&\frac{2}{5}(4n+2m)\sqrt{2}+\frac{1}{7}\sqrt{14}(8n+4m)+\frac{1}{42}\sqrt{462}(16n+4m)\\&\frac{4}{7}\sqrt{3}n-\frac{1}{3}\sqrt{30}m-2n-\frac{22}{9}m+\frac{1}{28}\sqrt{182}(8n+4m)+\\&\frac{1}{8}\sqrt{14}(-8n-4m).\end{aligned}$$

Proof. Let $e_{i,j}$ denotes the number of edges of the chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$ with $i = S_{x_1}$ and $j = S_{x_2}$. It is easy to see that the summation of degree of edge endpoints of given graph has nine edge types $e_{5,5}$, $e_{5,7}$, $e_{6,7}$, $e_{6,8}$, $e_{7,7}$, $e_{7,8}$, $e_{8,8}$, $e_{8,9}$ and $e_{9,9}$ that are shown in Table 4.9. The fourth atom-bound connectivity index ABC_4 is defined as:

$$ABC_4(G) = \sum_{x_1x_2\in E(G)} \sqrt{\frac{S_{x_1}+S_{x_2}-2}{S_{x_1}\times S_{x_2}}},$$

this implies that

$$\begin{aligned}ABC_4(G) &= e_{5,5}\sqrt{\frac{5+5-2}{5\times5}}+e_{5,7}\sqrt{\frac{5+7-2}{5\times7}}+e_{6,7}\sqrt{\frac{6+7-2}{6\times7}}+\\&e_{6,8}\sqrt{\frac{6+8-2}{6\times8}}+e_{7,7}\sqrt{\frac{7+7-2}{7\times7}}+e_{7,8}\sqrt{\frac{7+8-2}{7\times8}}+\\&e_{8,8}\sqrt{\frac{8+8-2}{8\times8}}+e_{8,9}\sqrt{\frac{8+9-2}{8\times9}}+e_{9,9}\sqrt{\frac{9+9-2}{9\times9}}.\end{aligned}$$

By using Table 4.9, we obtain

$$\begin{aligned} ABC_4(G) &= (4n+2m)\sqrt{\tfrac{5+5-2}{5\times5}} + (8n+4m)\sqrt{\tfrac{5+7-2}{5\times7}} + \\ &\quad (40mn+16n+4m)\sqrt{\tfrac{6+7-2}{6\times7}} + (20mn-4n-4m)\sqrt{\tfrac{6+8-2}{6\times8}} + \\ &\quad (10mn+2n)\sqrt{\tfrac{7+7-2}{7\times7}} + (8n+4m)\sqrt{\tfrac{7+8-2}{7\times8}} + \\ &\quad (18mn-8n-4m)\sqrt{\tfrac{8+8-2}{8\times8}} + (4mn-4m)\sqrt{\tfrac{8+9-2}{8\times9}} + \\ &\quad (mn-m)\sqrt{\tfrac{9+9-2}{9\times9}}. \end{aligned}$$

After simplification, we obtain the desired result. □

Theorem 4.3.5. *The fifth geometric-arithmetic index GA_5 of the chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$ is given by*

$$\begin{aligned} GA_5(G) &= \left(\frac{80}{7}\sqrt{3} + 29 + \frac{80}{13}\sqrt{42} + \frac{48}{17}\sqrt{2}\right) mn - 2n - 3m + \\ &\quad \frac{1}{6}\sqrt{35}\,(8n+4m) + \frac{2}{13}\sqrt{42}\,(16n+4m) + \frac{4}{15}\sqrt{14}\,(8n+4m) + \\ &\quad \frac{4}{7}\sqrt{3}\,(-4n-4m) - \frac{48}{17}\sqrt{2}m. \end{aligned}$$

Proof. Let $e_{i,j}$ denotes the number of edges of the chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$ with $i = S_{x_1}$ and $j = S_{x_2}$. It is easy to see that the summation of degree of edge endpoints of given graph has nine edge types $e_{5,5}$, $e_{5,7}$, $e_{6,7}$, $e_{6,8}$, $e_{7,7}$, $e_{7,8}$, $e_{8,8}$, $e_{8,9}$ and $e_{9,9}$ that are shown in Table 4.9. The fifth geometric-arithmetic index GA_5 is defined as

$$GA_5(G) = \sum_{x_1x_2\in E(G)} \frac{2\sqrt{S_{x_1}\times S_{x_2}}}{S_{x_1}+S_{x_2}},$$

this implies that

$$\begin{aligned} GA_5(G) &= e_{5,5}\frac{2\sqrt{5\times 5}}{5+5} + e_{5,7}\frac{2\sqrt{5\times 7}}{5+7} + e_{6,7}\frac{2\sqrt{6\times 7}}{6+7} + \\ & e_{6,8}\frac{2\sqrt{6\times 8}}{6+8} + e_{7,7}\frac{2\sqrt{7\times 7}}{7+7} + e_{7,8}\frac{2\sqrt{7\times 8}}{7+8} + \\ & e_{8,8}\frac{2\sqrt{8\times 8}}{8+8} + e_{8,9}\frac{2\sqrt{8\times 9}}{8+9} + e_{9,9}\frac{2\sqrt{9\times 9}}{9+9}. \end{aligned}$$

By using Table 4.9, we obtain

$$\begin{aligned} GA_5(G) &= (4n+2m)\frac{2\sqrt{5\times 5}}{5+5} + (8n+4m)\frac{2\sqrt{5\times 7}}{5+7} + (40mn+16n+ \\ & 4m)\frac{2\sqrt{6\times 7}}{6+7} + (20mn-4n-4m)\frac{2\sqrt{6\times 8}}{6+8} + (10mn+ \\ & 2n)\frac{2\sqrt{7\times 7}}{7+7} + (8n+4m)\frac{2\sqrt{7\times 8}}{7+8} + (18mn-8n-4m)\frac{2\sqrt{8\times 8}}{8+8} + \\ & (4mn-4m)\frac{2\sqrt{8\times 9}}{8+9} + (mn-m)\frac{2\sqrt{9\times 9}}{9+9}. \end{aligned}$$

After simplification, we obtain the desired result. □

We compute hyper-Zagreb index $HM(G)$, first multiple Zagreb index $PM_1(G)$, second multiple Zagreb index $PM_2(G)$, Zagreb polynomials $M_1(G,x)$, $M_2(G,x)$ for chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$ in the following theorem.

Theorem 4.3.6. *Let G be a chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$. Then*

1. $HM(G) = 1500n - 48m + 2688mn$

2. $PM_1(G) = 2^{33mn+10n-m} \times 3^{33mn+2n-5m} \times 5^{60mn+20n+4m}$

3. $PM_2(G) = 2^{60mn+28n+8m} \times 3^{126mn+24n-6m}$

4. $M_1(G,x) = (4n + 2m)x^4 + (60mn + 20n + 4m)x^5 +$

$(33mn + 26n - 5m)x^6$

5. $M_2(G,x) = (4n + 2m)x^4 + (60mn + 20n + 4m)x^6$

$+ (33mn + 26n - 5m)x^9$.

Proof. Let G be a chemical structures of the conductive 2D MOFs $Cu_3(HITP)_2[m,n]$. The edge set $E(G)$ divided into three edge partitions based on degree of end vertices. The first edge partition $E_1(G)$ contains $4n + 2m$ edges x_1x_2, where $d_{x_1} = d_{x_2} = 2$. The second edge partition $E_2(G)$ contains $60mn + 20n + 4m$ edges x_1x_2, where $d_{x_1} = 2$, $d_{x_2} = 3$. The third edge partition $E_3(G)$ contains $33mn + 2n - 5m$ edges x_1x_2, where $d_{x_1} = 3$, $d_{x_2} = 3$. It is easy to see that $|E_1(G)| = e_{2,2}$, $|E_2(G)| = e_{2,3}$ and $|E_3(G)| = e_{3,3}$. Since,

$$\begin{aligned}
HM(G) &= \sum_{x_1x_2 \in E(G)} (d_{x_1} + d_{x_2})^2 \\
&= \sum_{x_1x_2 \in E_1(G)} [d_{x_2}]^2 + \sum_{x_1x_2 \in E_2(G)} [d_{x_1} + d_{x_2}]^2 + \sum_{x_1x_2 \in E_3(G)} [d_{x_1} + d_{x_2}]^2 \\
&= 16|E_1(G)| + 25|E_2(G)| + 36|E_3(G)| \\
&= 16(4n + 2m) + 25(60mn + 20n + 4m) + 36(33mn + 2n - 5m),
\end{aligned}$$

this implies that

$$HM(G) = 1500n - 48m + 2688mn.$$

We have

$$
\begin{aligned}
PM_1(G) &= \prod_{x_1x_2\in E(G)} (d_{x_1}+d_{x_2}) \\
&= \prod_{x_1x_2\in E_1(G)} (d_{x_1}+d_{x_2}) \times \prod_{x_1x_2\in E_2(G)} (d_{x_1}+d_{x_2}) \times \prod_{x_1x_2\in E_3(G)} (d_{x_1}+d_{x_2}) \\
&= 4^{|E_1(G)|} \times 5^{|E_2(G)|} \times 6^{|E_3(G)|} \\
&= 4^{4n+2m} \times 5^{60mn+20n+4m} \times 6^{33mn+2n-5m} \\
&= 2^{33mn+10n-m} \times 3^{33mn+2n-5m} \times 5^{60mn+20n+4m},
\end{aligned}
$$

and

$$
\begin{aligned}
PM_2(G) &= \prod_{x_1x_2\in E(G)} (d_{x_1}\times d_{x_2}) \\
&= \prod_{x_1x_2\in E_1(G)} (d_{x_1}\times d_{x_2}) \times \prod_{x_1x_2\in E_2(G)} (d_{x_1}\times d_{x_2}) \times \prod_{x_1x_2\in E_3(G)} (d_{x_1}\times d_{x_2}) \\
&= 4^{|E_1(G)|} \times 6^{|E_2(G)|} \times 9^{|E_3(G)|} \\
&= 4^{4n+2m} \times 6^{60mn+20n+4m} \times 9^{33mn+2n-5m} \\
&= 2^{60mn+28n+8m} \times 3^{126mn+24n-6m}.
\end{aligned}
$$

We also obtain that

$$
\begin{aligned}
M_1(G,x) &= \sum_{x_1x_2\in E(G)} x^{(d_{x_1}+d_{x_2})} \\
&= \sum_{x_1x_2\in E_1(G)} x^{(d_{x_1}+d_{x_2})} + \sum_{x_1x_2\in E_2(G)} x^{(d_{x_1}+d_{x_2})} + \sum_{x_1x_2\in E_3(G)} x^{(d_{x_1}+d_{x_2})} \\
&= \sum_{x_1x_2\in E_1(G)} x^4 + \sum_{x_1x_2\in E_2(G)} x^5 + \sum_{x_1x_2\in E_3(G)} x^6 \\
&= |E_1(G)|x^4 + |E_1(G)|x^5 + |E_1(G)|x^6 \\
&= (4n+2m)\,x^4 + (60mn+20n+4m)\,x^5 + (33mn+26n-5m)\,x^6,
\end{aligned}
$$

and

$$\begin{aligned}
M_2(G,x) &= \sum_{x_1x_2\in E(G)} x^{(d_{x_1}\times d_{x_2})} \\
&= \sum_{x_1x_2\in E_1(G)} x^{(d_{x_1}\times d_{x_2})} + \sum_{x_1x_2\in E_2(G)} x^{(d_{x_1}\times d_{x_2})} + \sum_{x_1x_2\in E_3(G)} x^{(d_{x_1}\times d_{x_2})} \\
&= \sum_{x_1x_2\in E_1(G)} x^4 + \sum_{x_1x_2\in E_2(G)} x^6 + \sum_{x_1x_2\in E_3(G)} x^9 \\
&= |E_1(G)|x^4 + |E_1(G)|x^6 + |E_1(G)|x^9 \\
&= (4\,n + 2\,m)\,x^4 + (60\,mn + 20\,n + 4\,m)\,x^6 + (33\,mn + 26\,n - 5\,m)\,x^9.
\end{aligned}$$

This completes the proof. □

4.4 Line graph and line graph of subdividion of chemical structures of the conductive 2D MOFs

Figure 4.5, represents the unit cell of line graph of chemical structures of the conductive 2D MOFs.

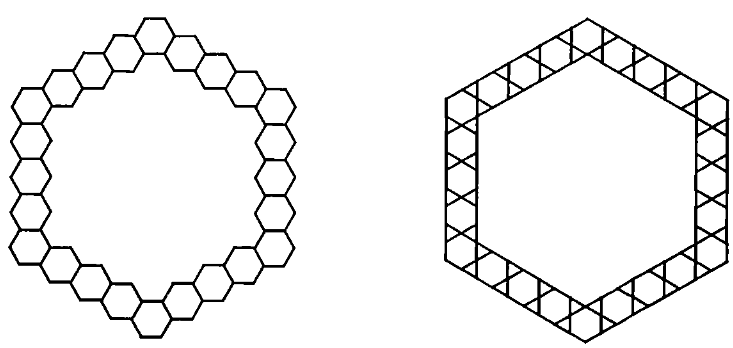


Figure 4.5: The unit cell of graph G and its line graph.

4.4.1 Topological indices of $m \times n$ sheet of G_L

Let G_L be the line graph of chemical structures of the conductive 2D MOFs. The unit cell of G_L contains one main hexagon with minor hexagons is shown in Figure 4.5. The unit cells of G_L can be arranged either linearly or in a sheet form. A linear arrangement with n unit cells of G_L is called n chain of unit cell of G_L, $m \times n$ sheet of G_L is obtained by arrangements of mn unit cells of G_L into m rows and n columns. A $m \times n$ sheet of G_L contains $93mn + m + 26n$ vertices among of which $2m + 2n$ vertices are of degree 2, $60mn + 20n + 4m$ vertices are of degree 3 and $33mn + 2n - 5m$ vertices are of degree 4. By handshaking lemma, the number of edges of $m \times n$ sheet of G_L are $156mn + 38n - 2m$. In the following theorem, we determine the first Zagreb index M_1, Narumi-Katayama index NK and first multiplicative Zagreb index PM_1 for graph G_L.

Theorem 4.4.1. *Let G_L be a $m \times n$ sheet with m is the number of main hexagons in any row and n is the number of main hexagons in any column. Then*

1. $M_1(G_L) = 1068mn - 36m + 228n$
2. $NK(G_L) = 2^{66mn-8m+8n} \cdot 3^{60mn+4m+20n}$
3. $PM_1(G_L) = 2^{132mn-16m+16n} \cdot 3^{120mn+8m+40n}$.

Proof. Let $n_{x_1}^{G_L}$ denotes the number of vertices of degree d_{x_1} in graphs G_L. In G_L, the number of vertices of degree 2,3 and 4 are: $n_2^{G_L} = 2m + 2n$, $n_3^{G_L} = 60mn + 20n + 4m$, and $n_4^{G_L} = 33mn + 2n - 5m$. Putting these values in equation (2.6) and equation (2.4), we get the required results. □

We now determine Randić index $R(G_L)$, reciprocal Randić index $RR(G_L)$, second Zagreb index $M_2(G_L)$, second multiplicative Zagreb index

$PM_2(G_L)$, hyper Zagreb index $HM(G_L)$, sum-connectivity index $SC(G_L)$ and modified first multiplicative Zagreb index $\pi_1^*(G_L)$.

Theorem 4.4.2. *Let G_L be a $m \times n$ sheet with m is the number of main hexagons in any row and n is the number of main hexagons in any column. Then*

1. $R(G_L) = \left(\frac{139}{6} + \frac{40}{3}\sqrt{3}\right) mn + \left(\frac{2}{3}\sqrt{6} - \frac{7}{6}\right) m + \left(\frac{4}{3}\sqrt{6} + 5 + \frac{8}{3}\sqrt{3}\right) n$

2. $RR(G_L) = \left(254 + 160\sqrt{3}\right) mn + \left(4\sqrt{6} - 28\right) m + \left(8\sqrt{6} + 32\sqrt{3} + 38\right) n$

3. $M_2(G_L) = 1826mn - 100m + 338n$

4. $PM_2(G_L) = 2^{264mn-36m+24n} \cdot 3^{180mn+12m+60n}$

5. $HM(G_L) = 7384mn - 396m + 1376n$

6. $SC(G_L) = (\frac{25}{3}\sqrt{6}+\frac{80}{7}\sqrt{7}+\frac{13}{2}\sqrt{2})mn+(\frac{16}{7}\sqrt{7}+\frac{8}{5}\sqrt{5}-\sqrt{2}+3\sqrt{6})n+(\frac{2}{3}\sqrt{6}+\frac{4}{5}\sqrt{5} - \frac{5}{2}\sqrt{2})m$

7. $\pi_1^*(G_L) = 2^{128mn+6n-26m} \cdot 3^{50mn+18n+4m} \cdot 5^{4m+8n} \cdot 7^{80mn+16n}$.

Proof. Let $e_{x_1,x_2}^{G_L}$ denotes the number of edges in the edge partition $E_{x_1,x_2}^{G_L}$ with the degree of end vertices are d_{x_1} and d_{x_2}. This implies that $e_{2,3}^{G_L} = 8n + 4m$, $e_{3,3}^{G_L} = 50mn + 18n + 4m$, $e_{3,4}^{G_L} = 80mn + 16n$ and $e_{4,4}^{G_L} = 26mn - 4n - 10m$. Putting these values in equation (2.2), for $\alpha = \frac{-1}{2}, \frac{1}{2}, 1$, and after simplification we obtain the Randić index, reciprocal Randić index and second Zagreb index, respectively. By Using $\alpha = 2, \frac{-1}{2}$ and $e_{2,3}^{G_L}, e_{3,3}^{G_L}, e_{3,4}^{G_L}, e_{4,4}^{G_L}$ in equation (2.3), we get the hyper Zagreb index and sum-connectivity index, respectively. The second multiplicative Zagreb index $PM_2(G_L)$ and modified first multiplicative Zagreb index $\pi_1^*(G)$ can be obtained by putting the values of the edge partition of the graph G_L in the equations (2.13) and (2.14). This completes the proof. □

We now compute the augmented Zagreb index AZ, Harmonic index H, atom-bond connectivity index ABC and geometric-arithmetic index GA for G_L.

Theorem 4.4.3. *Let G_L be a $m \times n$ sheet with m is the number of main hexagons in any row and n is the number of main hexagons in any column. Then, we obtain the following*

1. $AZ(G_L) = \frac{46839347}{21600}mn - \frac{48413}{432}m + \frac{44751247}{108000}n$
2. $H(G_L) = \frac{1933}{42}mn + \frac{13}{30}m + \frac{447}{35}n$
3. $ABC(G_L) = \left(\frac{100}{3} + \frac{40}{3}\sqrt{15} + \frac{13}{2}\sqrt{6}\right) mn + \left(12 + \frac{8}{3}\sqrt{15} + 4\sqrt{2} - \sqrt{6}\right) n + \left(2\sqrt{2} - \frac{5}{2}\sqrt{6} + \frac{8}{3}\right) m$
4. $GA(G_L) = \left(76 + \frac{320}{7}\sqrt{3}\right) mn + \left(\frac{16}{5}\sqrt{6} + 14 + \frac{64}{7}\sqrt{3}\right) n + \left(\frac{8}{5}\sqrt{6} - 6\right) m.$

Proof. By using the values the edge partitions for the graph G_L in the equations (2.11), (2.5), (2.7) and (2.9), after simple calculation and simplification, we obtain the required results. □

Let denote the fourth version of ABC index and fifth version of GA index as ABC_4 and GA_5, respectively.

Theorem 4.4.4. *Let G_L be a $m \times n$ sheet with m is the number of main hexagons in any row and n is the number of main hexagons in any column. The ABC_4*

index and $GA_5(G)$ *of graph* G_L *are given as follows.*

$$\begin{aligned} ABC_4(G_L) &= (9\sqrt{2} + \frac{20}{3}\sqrt{6} + \frac{8}{7}\sqrt{26} + \frac{2}{11}\sqrt{2090} + \frac{6}{35}\sqrt{70} + \frac{18}{77}\sqrt{3542} + \\ &\frac{4}{15}\sqrt{7} + \frac{8}{55}\sqrt{110} + \frac{1}{15}\sqrt{435})mn + (\frac{2}{9}\sqrt{78} - \frac{6}{35}\sqrt{70} + \\ &\frac{2}{15}\sqrt{170} + \frac{2}{65}\sqrt{2730} + \frac{8}{39}\sqrt{65} - \frac{1}{15}\sqrt{435} + \frac{6}{5}\sqrt{2} - \frac{4}{15}\sqrt{7} + \\ &\frac{2}{91}\sqrt{26} - \frac{8}{55}\sqrt{110} - \frac{2}{55}\sqrt{2090} - \frac{1}{77}\sqrt{3542} + \frac{10}{91}\sqrt{182})m + \\ &(\frac{4}{9}\sqrt{78} + \frac{4}{3}\sqrt{6} + \frac{4}{15}\sqrt{170} - \frac{22}{91}\sqrt{26} + \frac{16}{39}\sqrt{65} + \frac{21}{5}\sqrt{2} - \\ &\frac{8}{77}\sqrt{3542} + \frac{4}{65}\sqrt{2730} - \frac{2}{55}\sqrt{2090} + \frac{20}{91}\sqrt{182})n \end{aligned}$$

and

$$\begin{aligned} GA_5(G_L) &= (\frac{80}{11}\sqrt{30} + \frac{40}{21}\sqrt{110} + 48 + \frac{72}{25}\sqrt{154} + \frac{8}{29}\sqrt{210} + \frac{4}{13}\sqrt{165} + \\ &\frac{32}{31}\sqrt{15})mn + (\frac{8}{5}\sqrt{6} - \frac{32}{31}\sqrt{15} + \frac{24}{19}\sqrt{10} + \frac{8}{23}\sqrt{130} + \frac{12}{11}\sqrt{13} - \\ &\frac{4}{13}\sqrt{165} + \frac{8}{27}\sqrt{182} - \frac{8}{29}\sqrt{210} - 2 - \frac{8}{21}\sqrt{110} - \frac{16}{25}\sqrt{154} + \\ &\frac{1}{3}\sqrt{143})m + (\frac{16}{5}\sqrt{6} + 2 + \frac{16}{11}\sqrt{30} + \frac{16}{27}\sqrt{182} + \frac{48}{19}\sqrt{10} + \\ &\frac{2}{3}\sqrt{143} + \frac{24}{11}\sqrt{13} - \frac{8}{21}\sqrt{110} - \frac{32}{25}\sqrt{154} + \frac{16}{23}\sqrt{130})n. \end{aligned}$$

Proof. Let $m_{a,b}^{G_L}$ denotes the number of edges of edge partition of G_L with $a = S_{x_1}$ and $b = S_{x_2}$, where S_{x_1} is the sum degrees of neighbor vertices of x_1. It is easy to see that there fifteen such type of edge partitions $m_{a,b}^{G_L}$ which are as follows: $m_{6,9}^{G_L} = 4m + 8n, m_{9,10}^{G_L} = 4m + 8n, m_{9,13}^{G_L} = 4m + 8n, m_{10,10}^{G_L} = 30mn + 4m + 14n, m_{10,11}^{G_L} = 20mn - 4m - 4n, m_{10,12}^{G_L} = 40mn + 8n, m_{10,13}^{G_L} = 4m + 8n, m_{11,13}^{G_L} = 4m+8n, m_{11,14}^{G_L} = 36mn-8m-16n, m_{11,15}^{G_L} = 4mn+4m, m_{13,14}^{G_L} = 4m+8n, m_{14,14}^{G_L} = 16mn-4m-12n, m_{14,15}^{G_L} = 4mn-4m, m_{15,15}^{G_L} = 2mn-2m$ and $m_{15,16}^{G_L} = 4mn-4m$.

For the ABC_4 index of graph G_L, we have

$$ABC_4(G_L) = \sum_{x_1x_2 \in E(G_L)} \sqrt{\frac{S_{x_1} + S_{x_2} - 2}{S_{x_1}S_{x_2}}}$$

$$= m_{6,9}^{G_L}\sqrt{\frac{6+9-2}{6\times 9}} + m_{9,10}^{G_L}\sqrt{\frac{9+10-2}{9\times 10}} + m_{9,13}^{G_L}\sqrt{\frac{9+13-2}{9\times 13}}$$
$$+ m_{10,10}^{G_L}\sqrt{\frac{10+10-2}{10\times 10}} + m_{10,11}^{G_L}\sqrt{\frac{10+11-2}{10\times 11}} + m_{10,12}^{G_L}\sqrt{\frac{10+12-2}{10\times 12}}$$
$$+ m_{10,13}^{G_L}\sqrt{\frac{10+13-2}{10\times 13}} + m_{11,13}^{G_L}\sqrt{\frac{11+13-2}{11\times 13}} + m_{11,14}^{G_L}\sqrt{\frac{11+14-2}{11\times 14}}$$
$$+ m_{11,15}^{G_L}\sqrt{\frac{11+15-2}{11\times 15}} + m_{13,14}^{G_L}\sqrt{\frac{13+14-2}{13\times 14}} + m_{14,14}^{G_L}\sqrt{\frac{14+14-2}{14\times 14}}$$
$$+ m_{14,15}^{G_L}\sqrt{\frac{14+15-2}{14\times 15}} + m_{15,15}^{G_L}\sqrt{\frac{15+15-2}{15\times 15}} + m_{15,16}^{G_L}\sqrt{\frac{15+16-2}{15\times 16}}$$

$$= (4m+8n)\sqrt{\frac{13}{54}} + (4m+8n)\sqrt{\frac{17}{90}} + (4m+8n)\sqrt{\frac{20}{117}}$$
$$+ (30mn+4m+14n)\sqrt{\frac{18}{100}} + (20mn-4m-4n)\sqrt{\frac{19}{110}} + (40mn+8n)\sqrt{\frac{20}{120}}$$
$$+ (4m+8n)\sqrt{\frac{21}{130}} + (4m+8n)\sqrt{\frac{22}{143}} + (36mn-8m-16n)\sqrt{\frac{23}{154}}$$
$$+ (4mn+4m)\sqrt{\frac{24}{165}} + (4m+8n)\sqrt{\frac{25}{182}} + (16mn-4m-12n)\sqrt{\frac{26}{196}}$$
$$+ (4mn-4m)\sqrt{\frac{27}{210}} + (2mn-2m)\sqrt{\frac{28}{225}} + (4mn-4m)\sqrt{\frac{29}{240}},$$

and for the GA_5 of graph G_L, we have

$$
\begin{aligned}
GA_5(G_L) &= \sum_{x_1x_2\in E(G_L)} 2\frac{\sqrt{S_{x_1}S_{x_2}}}{S_{x_1}+S_{x_2}} \\
&= m_{6,9}^{G_L}2\frac{\sqrt{6\times 9}}{6+9} + m_{9,10}^{G_L}2\frac{\sqrt{9\times 10}}{9+10} + m_{9,13}^{G_L}2\frac{\sqrt{9\times 13}}{9+13} + \\
& m_{10,10}^{G_L}2\frac{\sqrt{10\times 10}}{10+10} + m_{10,11}^{G_L}2\frac{\sqrt{10\times 11}}{10+11} + m_{10,12}^{G_L}2\frac{\sqrt{10\times 12}}{10+12} + \\
& m_{10,13}^{G_L}2\frac{\sqrt{10\times 13}}{10+13} + m_{11,13}^{G_L}2\frac{\sqrt{11\times 13}}{11+13} + m_{11,14}^{G_L}2\frac{\sqrt{11\times 14}}{11+14} + \\
& m_{11,15}^{G_L}2\frac{\sqrt{11\times 15}}{11+15} + m_{13,14}^{G_L}2\frac{\sqrt{13\times 14}}{13+14} + m_{14,14}^{G_L}2\frac{\sqrt{14\times 14}}{14+14} + \\
& m_{14,15}^{G_L}2\frac{\sqrt{14\times 15}}{14+15} + m_{15,15}^{G_L}2\frac{\sqrt{15\times 15}}{15+15} + m_{15,16}^{G_L}2\frac{\sqrt{15\times 16}}{15+16}
\end{aligned}
$$

$$
\begin{aligned}
= {} & 2(4m+8n)\frac{\sqrt{54}}{15} + 2(4m+8n)\frac{\sqrt{90}}{19} + 2(4m+8n)\frac{\sqrt{117}}{22} + \\
& 2(30mn+4m+14n)\frac{\sqrt{100}}{20} + 2(20mn-4m-4n)\frac{\sqrt{110}}{21} + 2(40mn + \\
& 8n)\frac{\sqrt{120}}{22} + 2(4m+8n)\frac{\sqrt{130}}{23} + 2(4m+8n)\frac{\sqrt{143}}{24} + \\
& 2(36mn-8m-16n)\frac{\sqrt{154}}{25} + 2(4mn+4m)\frac{\sqrt{165}}{26} + 2(4m+8n)\frac{\sqrt{182}}{27} + \\
& 2(16mn-4m-12n)\frac{\sqrt{196}}{28} + 2(4mn-4m)\frac{\sqrt{210}}{29} + 2(2mn-2m)\frac{\sqrt{225}}{30} + \\
& 2(4mn-4m)\frac{\sqrt{240}}{31}.
\end{aligned}
$$

After simplification, we obtain the desired results.

This completes the proof. □

We now compute Zagreb polynomials $M_1(G_L,x)$ and $M_2(G_L,x)$ for the graph G_L by using the equations (2.15,2.16) and the values of edge partition which are already mentioned in Theorem 4.4.2.

Theorem 4.4.5. *The Zagreb polynomials $M_1(G_L,x)$ and $M_2(G_L,x)$ for graph*

G_L are given as follows:

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

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

4.4.2 Topological indices of $m \times n$ sheet of G_{PL}

Let G_{PL} be the line graph of subdivision chemical structures of the conductive 2D MOFs. The unit cell of G_{PL} contains one main hexagon with minor hexagons is shown in Figure 4.6. The unit cells of G_{PL} can be arranged either linearly or in a sheet form. A linear arrangement with n unit cells of G_{PL} is called n chain of unit cell of G_{PL}, $m \times n$ sheet of G_{PL} is obtained by arrangements of mn unit cells of G_{PL} into m rows and n columns. A $m \times n$ sheet of G_{PL} contains total number of vertices are $186mn + 52n + 2m$. It is easy to see that there are $n_2 = |V_2| = 60mn + 28n + 8m$ and $n_3 = |V_3| = 126mn + 24n - 6m$. By Handshaking Lemma, total number of edges of $m \times n$ sheet of G_{PL} are $249mn + 64n - m$.

Similar to Theorem 4.4.1, we obtain the following.

Theorem 4.4.6. *Let G_{PL} be a $m \times n$ sheet with m is the number of main hexagons in any row and n is the number of main hexagons in any column. Then*

1. $M_1(G_{PL}) = 1374mn - 22m + 328n$

2. $NK(G_{PL}) = 2^{60mn+28n+8m} \cdot 3^{126mn+24n-6m}$

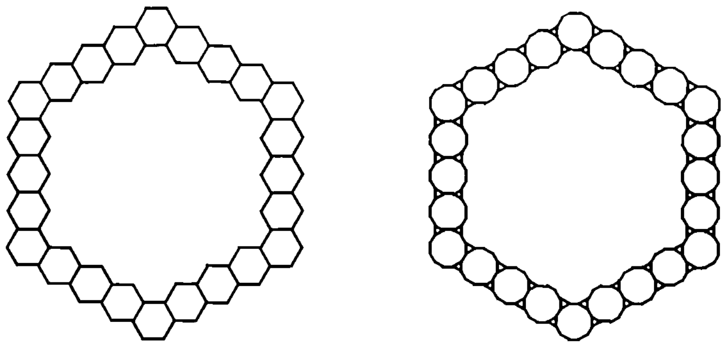


Figure 4.6: The unit cell of graph G and line graph of its subdivision.

3. $PM_1(G)(G_{PL}) = 2^{120mn+56n+16m} \cdot 3^{252mn+48n-12m}$.

Proof. Let $n_{x_1}^{G_{PL}}$ denotes the number of vertices of degree d_{x_1} in graphs G_{PL}. It is easy to see that $n_2^{G_{PL}} = 60mn + 28n + 8m$ and $n_3^{G_{PL}} = 126mn + 24n - 6m$. Putting these values in equation (2.6) and equation (2.4), we obtain the required results. □

Similar to Theorem 4.4.2, we obtain the following result.

Theorem 4.4.7. *Let G_{PL} be a $m \times n$ sheet with m is the number of main hexagons in any row and n is the number of main hexagons in any column. Then*

1. $R(G_{PL}) = \left(68 + 10\sqrt{6}\right) mn + \left(\frac{53}{3} + \frac{10}{3}\sqrt{6}\right) n + \left(-\frac{2}{3} + \frac{2}{3}\sqrt{6}\right) m$

2. $RR(G_{PL}) = \left(537 + 60\sqrt{6}\right) mn + \left(-21 + 4\sqrt{6}\right) m + \left(20\sqrt{6} + 114\right) n$

3. $M_2(G_{PL}) = 1911mn - 51m + 426n$

4. $PM_2(G_{PL}) = 2^{120mn+16m+56n} \cdot 3^{378mn+72n-18m}$

5. $HM(G_{PL}) = 7704mn - 200m + 1724n$

6. $SC(G_{PL}) = (15+12\sqrt{5}+\frac{53}{2}\sqrt{6})mn+(\frac{13}{3}\sqrt{6}+9+4\sqrt{5})n+(\frac{4}{5}\sqrt{5}+3-\frac{11}{6}\sqrt{6})m$

7. $\pi_1^*(G_{PL}) = 2^{219mn+m+62n} \cdot 3^{159mn+26n-11m} \cdot 5^{60mn+20n+4m}$.

Proof. Let $e_{x_1,x_2}^{G_{PL}}$ denotes the number of edges in the edge partition $E_{x_1,x_2}^{G_{PL}}$ with the degree of end vertices are d_{x_1} and d_{x_2}. This implies that $e_{2,2}^{G_{PL}} = 30mn+6m+18n$, $e_{2,3}^{G_{PL}} = 60mn + 20n + 4m$ and $e_{3,3}^{G_{PL}} = 159mn + 26n - 11m$. Putting these values in equation (2.1), for $\alpha = \frac{-1}{2}, 1, \frac{1}{2}$, and after simplification, we obtain values of Randić index, reciprocal Randić index and second Zagreb index, respectively. By using $\alpha = 2, \frac{-1}{2}$ and $e_{2,2}^{G_{PL}}, e_{2,3}^{G_{PL}}, e_{3,3}^{G_{PL}}$ in equation (2.2), we obtain the hyper Zagreb index and sum-connectivity index, respectively. The second multiplicative Zagreb index $PM_2(G_{PL})$ and modified first multiplicative Zagreb index $\pi_1^*(G_{PL})$ can be obtained by putting the values of the edge partition of the graph G_{PL} in the equation (2.13). This completes the proof. □

Similar to Theorem 4.4.3, we obtain the following result.

Theorem 4.4.8. *Let G_{PL} be the graph with m is the number of main hexagons in any row and n is the number of main hexagons in any column. Then the following holds:*

1. $AZ(G_{PL}) = \frac{161991}{64}mn - \frac{2899}{64}m + \frac{19205}{32}n$,

2. $H(G_{PL}) = 92mn + \frac{14}{15}m + \frac{77}{3}n$,

3. $ABC(G_{PL}) = \left(45\sqrt{2} + 106\right) mn + 5m\sqrt{2} - \frac{22}{3} + \left(19\sqrt{2} + \frac{52}{3}\right) n$,

4. $GA(G_{PL}) = \left(189 + 24\sqrt{6}\right) mn + \left(8\sqrt{6} + 44\right) n + \left(-5 + \frac{8}{5}\sqrt{6}\right) m$.

Proof. By using the values the edge partitions for the graph G_{PL} in the equations

(2.11), (2.5), (2.7) and (2.9), after simple calculation and simplification, we obtain the required results. □

Similar to Theorem 4.4.4, we obtain the following result.

Theorem 4.4.9. *The ABC_4 index and GA_5 index of graph G_{PL} are given as follows.*

$$\begin{aligned} ABC_4(G_{PL}) &= (3\sqrt{110}+12\sqrt{2}+\frac{20}{3}\sqrt{30}+\frac{236}{9}+\frac{5}{2}\sqrt{14})mn+ \\ &\quad (\frac{1}{2}\sqrt{6}-\frac{20}{3}+\frac{2}{5}\sqrt{35}+\frac{1}{2}\sqrt{14}+\frac{1}{5}\sqrt{110})m+ \\ &\quad (\sqrt{6}+\frac{4}{5}\sqrt{35}+\frac{12}{5}\sqrt{2}+\frac{3}{2}\sqrt{14}+\frac{4}{3}\sqrt{30}+\sqrt{110})n-\frac{8}{9}, \end{aligned}$$

and

$$\begin{aligned} GA_5(G_{PL}) &= (109+\frac{240}{13}\sqrt{10}+\frac{960}{17}\sqrt{2})mn+(-9+\frac{16}{9}\sqrt{5} \\ &\quad +\frac{16}{13}\sqrt{10})m+(20+\frac{32}{9}\sqrt{5}+\frac{80}{13}\sqrt{10}+\frac{192}{17}\sqrt{2})n. \end{aligned}$$

Proof. Let $m_{a,b}^{G_{PL}}$ denotes the number of edges of edge partition of G_{PL} with $a = S_{x_1}$ and $b = S_{x_2}$, where S_{x_1} is the sum degrees of neighbor vertices of x_1. It is easy to see that there seven such type of edge partitions $m_{a,b}^{G_{PL}}$ which are as follows: $m_{4,4}^{G_{PL}} = 2m+4n, m_{4,5}^{G_{PL}} = 4m+8n, m_{5,5}^{G_{PL}} = 30mn+6n, m_{5,8}^{G_{PL}} = 60mn+4m+20n, m_{8,8}^{G_{PL}} = 20mn+4m+12n, m_{8,9}^{G_{PL}} = 80mn+16n$ and $m_{9,9}^{G_{PL}} = 59mn-15m-2n$.

For the ABC_4 index of graph G_{PL}, we have

$$\begin{aligned}
ABC_4(G_{PL}) = &\sum_{x_1x_2\in E(G_{PL})} \sqrt{\frac{S_{x_1}+S_{x_2}-2}{S_{x_1}S_{x_2}}} \\
=&m_{4,4}^{G_{PL}}\sqrt{\frac{4+4-2}{4\times 4}} + m_{4,5}^{G_{PL}}\sqrt{\frac{4+5-2}{4\times 5}} + m_{5,5}^{G_{PL}}\sqrt{\frac{5+5-2}{5\times 5}} \\
+&m_{5,8}^{G_{PL}}\sqrt{\frac{5+8-2}{5\times 8}} + m_{8,8}^{G_{PL}}\sqrt{\frac{8+8-2}{8\times 8}} + m_{8,9}^{G_{PL}}\sqrt{\frac{8+9-2}{8\times 9}} \\
+&m_{9,9}^{G_{PL}}\sqrt{\frac{9+9-2}{9\times 9}} \\
=&(2m+4n)\sqrt{\frac{6}{16}} + (4m+8n)\sqrt{\frac{7}{20}} + (30mn+6n)\sqrt{\frac{8}{25}} \\
+&(60mn+4m+20n)\sqrt{\frac{11}{40}} + (20mn+4m+12n)\sqrt{\frac{14}{64}} \\
+&(80mn+16n)\sqrt{\frac{15}{72}} + (59mn-15m-2n)\sqrt{\frac{16}{81}}.
\end{aligned}$$

For the GA_5 index of graph G_{PL}, we obtain

$$\begin{aligned}
GA_5(G_{PL}) = &\sum_{x_1x_2\in E(G_{PL})} 2\frac{\sqrt{S_{x_1}S_{x_2}}}{S_{x_1}+S_{x_2}} \\
=&m_{4,4}^{G_{PL}}2\frac{\sqrt{4\times 4}}{4+4} + m_{4,5}^{G_{PL}}2\frac{\sqrt{4\times 5}}{4+5} + m_{5,5}^{G_{PL}}2\frac{\sqrt{5\times 5}}{5+5} + m_{5,8}^{G_{PL}}2\frac{\sqrt{5\times 8}}{5+8} \\
+&m_{8,8}^{G_{PL}}2\frac{\sqrt{8\times 8}}{8+8} + m_{8,9}^{G_{PL}}2\frac{\sqrt{8\times 9}}{8+9} + m_{9,9}^{G_{PL}}2\frac{\sqrt{9\times 9}}{9+9} \\
=&2(2m+4n)\frac{\sqrt{16}}{8} + 2(4m+8n)\frac{\sqrt{20}}{9} + 2(30mn+6n)\frac{\sqrt{25}}{10} \\
+&2(60mn+4m+20n)\frac{\sqrt{40}}{13} + 2(20mn+4m+12n)\frac{\sqrt{64}}{16} \\
+&2(80mn+16n)\frac{\sqrt{72}}{17} + 2(59mn-15m-2n)\frac{\sqrt{81}}{18}.
\end{aligned}$$

After simplification, we obtain the results as desired. This completes the proof. □

We compute Zagreb polynomials $M_1(G_{PL}, x)$ and $M_2(G_{PL}, x)$ for the graph G_{PL} by using the equations 2.15, 2.16 and the values of edge partition as in Theorem 4.4.7 in the following theorem.

Theorem 4.4.10. *The Zagreb polynomials $M_1(G_{PL}, x)$ and $M_2(G_{PL}, x)$ for the graph G_{PL} are given as follows.*

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

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

CHAPTER 5

DISTANCE BASED TOPOLOGICAL INDICES

In this chapter, distance among the vertices of graph and distance-based topological indices are focused. Distance calculator and distance based topological indices are computed using computer based algorithms for complete binary trees and for complete ternary trees.

5.1 Algorithmic Solution

This section is most prominent part of this chapter as it gives algorithms, that are implemented in computer to generate required outcomes. To start with algorithmic solutions, first question is about suitability of data-structure. Appropriate use of data-structure is the first key to get optimal results. In design phase Tree-of-Arrays is used as one of the classical data-structures. But in implementation phase 2D-Array is used for sake of efficiency. As algorithm design architecture both iteration and recursion is used, whereas to handle the distances of ancestors and descendants back-tracking is used as algorithmic design strategy.

To traverse between the levels of complete binary tree(CBT) and complete ternary tree(CTT) inline functions are used to probe the values of Left-Child, Right-Child, Mid-Child, and Parent vertices. In CBT Left(u) returns location $2 \times u$, Right(u) returns location $2 \times u + 1$ and Parent(u) returns location $\lfloor \frac{u}{2} \rfloor$. Similarly in CTT Left(u) returns location $3 \times u - 1$, Mid(u) returns location $3 \times u$, Right(u) returns location $3 \times u + 1$ and Parent(u) returns location $\lfloor \frac{u}{3} + 0.5 \rfloor$.

Algorithm 5 Distance-Calculator(m,H)

Input: The two positive integers m and H.
Output: 2D-array $Array$ that stores the count of all vertices which are at distance j for a vertex u.

$V \leftarrow \frac{(m^{H+1} - 1)}{(m - 1)}$
$Distance \leftarrow 2 \times H$
$Array[V][Distance] \leftarrow 0$
for $u \leftarrow 1$ to V
    $j \leftarrow 1$
    Fill(Array, u, root, j)
    Back-Track(Array, u, root, j)
return $Array$

Algorithm 6 Fill(Array, u, v, j)

Input: The 2D-array $Array$, three positive integers u,v, and j.
Output: $Array$ after adding distance counts in it.

if $(m = 2)$
    if (Right(u) $\leq V$)
        $Array[u][j] \leftarrow Array[u][j] + 2$
    if (Right(Right(u))$\leq V$)
        Apply recursive calls for all sub-child of u
if $(m = 3)$
    if (Right(u) $\leq V$)
        $Array[u][j] \leftarrow Array[u][j] + 3$
    if (Right(Right(u))$\leq V$)
        Apply recursive calls for all sub-child of u
return $Array$

Algorithm 7 Back-Track(Array, u, v, j)

Input: The 2D-array *Array*, three positive integers u, v, and j.

Output: *Array* after adding distance counts in it.

```
prev ← u
if (m = 2)
    while (Parent(u)≠ Right-Nodes())
        if (prev = Left(Parent(u)))
            Array[u][j] ← Array[u][j] + 1
            Call Fill for right sibling for j+1 distance
        prev, u ← Parent(u)
        j ← j + 1
    Array[u][j] ← Array[u][j] + 1
    Call Fill for right sibling for j+1 distance
if (m = 3)
    while (Parent(u)≠ Right-Nodes())
        if (prev = Left(Parent(u)))
            Array[u][j] ← Array[u][j] + 1
            Call Fill for mid and right siblings for j+1 distance
            Array[u][j] ← Array[u][j] + 1
        if (prev = Mid(Parent(u)))
            Array[u][j] ← Array[u][j] + 1
            Call Fill for right sibling for j+1 distance
        prev, u ← Parent(u)
        j ← j + 1
    if (prev = Left(Parent(u)))
        Array[u][j] ← Array[u][j] + 1
        Call Fill for mid and right siblings for j+1 distance
        Array[u][j] ← Array[u][j] + 1
    else
        Array[u][j] ← Array[u][j] + 1
        Call Fill for right sibling for j+1 distance
return Array
```

5.1.1 Description of Algorithm Distance-Calculator(m,H)

Algorithm takes two positive integers m and H, where m is the number of child for any internal vertex, and H is the height of the tree. Output of the algorithms is a 2D-Array that stores the count of all vertices which are at distance j for a vertex u. These distances are used to compute topological indices in Algorithm 2 and 3.

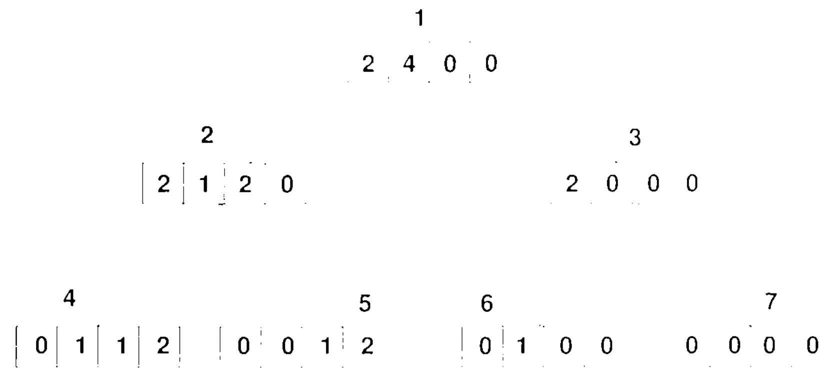


Figure 5.1: Output of distance calculator for $m = 2$ and $H = 2$ for CBT.

The Distance-Calculator algorithm requires two input parameter m and H to execute. Line 1,2 and 3, calculate the maximum vertex V, the maximum distance D and defines a 2d-Array $Array$, respectively. Line 4-7, execute a for loop to call Fill and Back-track part of the algorithm for all the vertices (from 1 to V) with root and distance $j = 1$. Line 8 return the output array $Array$.

The Fill algorithm requires 2D-Array $Array$, vertex v, vertex u and distance j as input parameters. Line 1-5, executes for binary tree when $m = 2$ where as Line 6-10 for ternary trees when $m = 3$. It works like Depth First Traversal. It count all the descendants of vertex u, from top to the bottom and add the distance in the array $Array$. For example, if there exist a vertex v at distance 2 from u, then it add 2 in $Array[u][2]$.

The Back-track requires 2D-Array $Array$, vertex v, vertex u and distance j as input parameters. For any input vertex u, it counts all the vertices v which are the descendants of the ancestors of u at right side. It starts with u, move top right vertex, add right sibling distance and all its ancestors distance in $Array$ for u, with the help of Fill algorithm. After that it keeps on moving up and right and repeat the process, until it reaches to the root or Right vertex of the tree. At the end, it updates all the vertices v distance from u in the $Array$, which are at the top and right from u in the tree.

Distance-Calculator executes Fill and Back-track for all the vertices in the tree. Fill calculates top to bottom distance for all the vertices. Back-track calculates the distance from left to right and bottom to top in the reverse direction, without including direct ancestors distance(already calculated in Fill). After executing Distance-Calculator, any to any vertex distance calculated in the *Array*. Tree-of-Arrays given in Figure-1 depicts the algorithmic results.

5.2 Time Complexity

Time Complexity depends on the varied values of independent variables (i.e) m and H. In order to calculate the exact executions of Fill and Back-track, a computer program was executed multiple times by variating the values of H and m. The number of counts are shown in Table 5.1. For calculating the cost of both algorithms empirically, asymptotic ranges were applied and we concluded that $T(m, H)$ for Fill cost is $\frac{m^{2H}-m^{H}}{m-1}$ and Back-Track cost is $\frac{m^{H+1}-m+mH-H}{m-1}$. For the sake of simplicity, we can say the upper-bounds for Fill and Back-track are $O(m^{2H})$ and $O(m^{H+1})$.

Table 5.1: Time Complexity for Algorithm Distance-Calculator(m,H).

H	m	**Fill**	**Back-track**	$\frac{m^{2H}-m^{H}}{m-1}$	$\frac{m^{H+1}-m+mH-H}{m-1}$
2	3	36	10	36	10
3	2	55	11	56	11
3	3	279	36	351	36
4	2	231	26	240	26
4	3	2439	116	3240	116
5	2	959	57	992	57
5	3	21960	358	29403	358

5.2.1 Description of Algorithm Wiener-Hosoya(m,H,Array)

The Wiener-Hosoya algorithm requires input parameters m, H and *Array* (calculated in Distance-Calculator algorithm) to execute. It calculates the Wiener

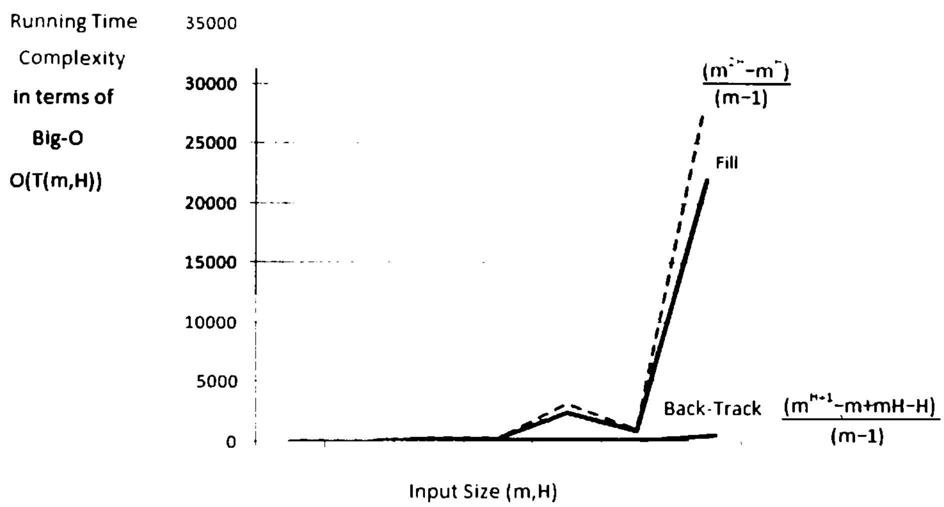


Figure 5.2: Time Complexity for Algorithm Distance-Calculator(m,H).

Algorithm 8 Wiener-Hosoya(m,H,Array)

Input: The two positive integers m, H and 2D-array $Array$.
Output: Weiner Index and Hosoya polynomial.

$V \leftarrow \frac{(m^{H+1}-1)}{(m-1)}$
$WeinerIndex \leftarrow 0$
for $j \leftarrow 1$ to $Distance$
    $HosoyaExp, HosoyaPol \leftarrow 0$
    for $i \leftarrow 1$ to V
        $WeinerIndex \leftarrow WeinerIndex + Array[i][j]$
        $HosoyaExp \leftarrow HosoyaExp + Array[i][j]$
    $HosoyaPol \leftarrow HosoyaPol + HosoyaExp \times x^j$
return $WeinerIndex, HosoyaPol$

Index, Hosoya polynomial and the Hosoya index for binary tree or ternary tree, by utilizing the required distance available in the *Array*.

Algorithm 9 Schultz-Indices(m,H)

Input: The two positive integers m and H.

Output: Two variables Sltz, and MSltz, containing Schultz index and modified Schultz index, respectively.

$V \leftarrow \frac{(m^{H+1}-1)}{(m-1)}$
$Distance \leftarrow 2 \times H$
$Array[V][Distance] \leftarrow 0$
$Sltz, MSltz \leftarrow 0$
for $u \leftarrow 1$ to V
    $j \leftarrow 1$
    Fill-Schultz(Array, u, root, j)
    Back-Track-Schultz(Array, u, root, j)
return $Sltz, MSltz$

Algorithm 10 Fill-Schultz(Array, u, v, j)

Input: The 2D-array *Array*, three positive integers u,v, and j.

Output: Return Sltz and MSltz after calculating Schultz index and modified Schultz index, from top to down distances.

if $(m = 2)$
  if (Right(u) $\leq V$)
    Calculate Schultz and Modified Schultz of all sub-child for j distance
  if (Right(Right(u))$\leq V$)
    Apply recursive calls for all sub-child of u as v
if $(m = 3)$
  if (Right(u) $\leq V$)
   Calculate Schultz and Modified Schultz of all sub-child for j distance
  if (Right(Right(u))$\leq V$)
    Apply recursive calls for all sub-child of u as v
return $Sltz, MSltz$

Algorithm 11 Back-Track-Schultz(Array, u, v, j)

Input: The 2D-array *Array*, three positive integers *u*,*v*, and *j*.

Output: Return Sltz and MSltz after calculating Schultz index and modified Schultz index, from bottom to up and left to right distances.

```
prev ← u
if (m = 2)
  while (Parent(u) ≠ Right-Nodes())
    if (prev = Left(Parent(u)))
      Calculate Schultz and Modified Schultz of right sibling for j+1 distance
      Call Fill-Schultz on right sibling for j+1 distance
    prev, u ← Parent(u)
    j ← j + 1
  Calculate Schultz and Modified Schultz of right sibling for j+1 distance
  Call Fill-Schultz on right sibling for j+1 distance
if (m = 3)
  while (Parent(u) ≠ Right-Nodes())
    if (prev = Left(Parent(u)))
      Calculate Schultz and Modified Schultz of mid and right sibling for j+1
          distance
      Call Fill-Schultz on mid and right sibling for j+1 distance
    if (prev = Mid(Parent(u)))
      Calculate Schultz and Modified Schultz of right sibling for j+1 distance
      Call Fill-Schultz on right sibling for j+1 distance
    prev, u ← Parent(u)
    j ← j + 1
  if (prev = Left(Parent(u)))
      Calculate Schultz and Modified Schultz of mid and right sibling for j+1
          distance
    Call Fill-Schultz on mid and right sibling for j+1 distance
  else
    Calculate Schultz and Modified Schultz of right sibling for j+1 distance
    Call Fill-Schultz on right sibling for j+1 distance
return Sltz, MSltz
```

5.2.2 Description of Algorithm Schultz-Indices(m,H)

The Schultz-Indices algorithm requires two input parameter m and H to execute. It works similar to the Distance-Calculator algorithm. It utilizes Fill-Schultz and Back-Track-Schultz algorithms. They are different from Fill and Back-track algorithms as both of them apply direct calculations for Schultz index and Modified-Schultz index in distance calculation (i.e, vertex u is connected to the vertex v with distance j), instead of updating the distance in *Array*. Schultz-Indices algorithm returns the Schultz index and Modified Schultz index as its output. Followings are the values of distance calculator for $m = 2$ and $H = 8$.

H	Weiner	Hosoya	Schultz	Modified Schultz
1	3	3.41	10	6
2	21	26.25	150	114
3	105	148.41	1262	1066
4	465	760.51	8286	7386
5	1953	3759.66	47550	43706
6	8001	18337.43	251262	235386
7	32385	88992.56	1257214	1192698
8	130305	431105.97	6055422	5795322

Followings are the values of distance calculator for $m = 3$ and $H = 5$.

H	Weiner	Hosoya	Schultz	Modified Schultz
1	6	6.93	24	15
2	78	102.1	708	564
3	780	1193.9	12048	10527
4	7260	13239.42	164328	149928
5	66066	144838.92	1999464	1867695

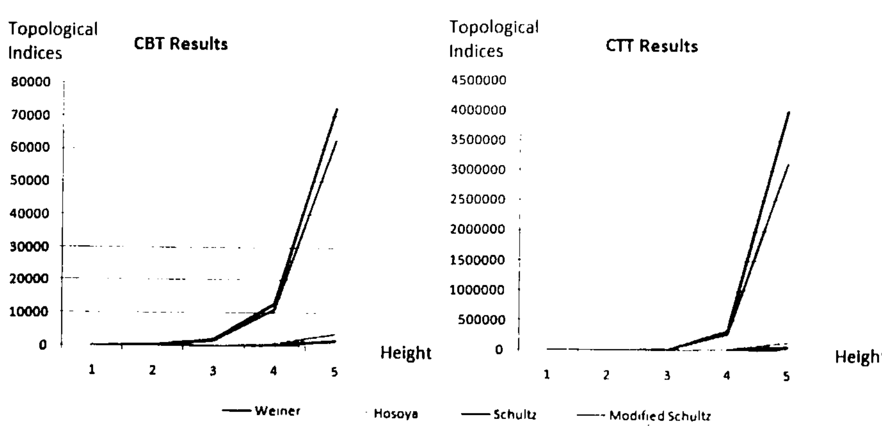


Figure 5.3: Comparison of Topological Indices.

5.3 Concluding Remarks

The outcomes of this research are helpful in two different ways. At first, it computes distance-based topological indices like Weiner index, Hosoya polynomial, Schultz index, and the modified-Schultz index of CBT and CTT for any height. Secondly distance calculator algorithm for CBT and CTT can be further modified to find the shortest path between any-to-any nodes of network graphs. By comparing the topological indices, it has been found that the value of the Schultz index is greater than the modified Schultz index, the modified Schultz index is greater than Hosoya polynomial for x [illegible] 1.1, and Hosoya polynomial is greater than Weiner index. Given algorithm is valid for any height as long as resources of computer supports, and its output can be used in plenty of computer applications like high-bandwidth routers, search applications, grammar checking applications, p2p programs, specialized image-signatures, video games, implementing efficient priority-queues, scheduling processes, cryptographic applications, memory management.

CHAPTER 6

CONCLUSION AND FUTURE WORKS

6.1 Conclusion

This study deepened the research by calculating topological indices algorithmically and mathematically for different graph families. Novelty of this study is that it provided the computer-based algorithms to compute eccentric topological indices, and distance based topological indices whereas degree based topological indices are calculated only mathematically for new graph families.

In the problem of zero divisor graphs with finite ring, construction algorithm is devised for zero divisor graphs containing commutative ring $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$ for prime numbers p_1, p_2 and q. Algorithm is designed and implemented on computer to explore the characteristics of the graph for vertex eccentric topological indices. Characteristics of zero divisor graphs containing commutative ring $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$ with prime p and q are also discovered. Algorithms are devised for edge eccentric topological indices for both zero divisor graphs containing commutative ring $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$ and zero divisor graph containing commutative ring $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$. Algorithmic results are compared with the mathematically calculated results.

In the problems related to line graphs and their subdivision for benzene ring in p-type surface and 2D conductive metallic organic framework $Cu_3(HITP)_2[m,n]$, degree based topological indices are calculated, namely, first general Zagreb index, general Randić connectivity index, general sum-connectivity index, atom-bond connectivity index, geometric-arithmetic index, forth atom-bond connectivity index, fifth geometric-arithmetic index, hyper-Zagreb index, first multiple Zagreb index, second multiple Zagreb index and Zagreb polynomials are calculated.

In the problem of complete binary tree and complete ternary tree, algorithm is experimented on computer by varying the domain values (m, H) to calculate any to any vertex distance among the nodes of tree. In this experiment different treatments are executed to find the distance based topological indices for m = 2, 3 with different heights varying 2 to 8. Outcomes of any-to-any distance table is utilized in further algorithms to calculate distance based topological indices including Weiner index, Hosoya index, Schultz index and modified Schultz index.

To conclude the hypothetical assumptions posed in research objectives following open problem and conjecture are framed on the basis of results in chapter 3, 4 and 5.

6.1.1 Open Problem

(i) Eccentric topological indices for zero divisor graphs containing commutative rings $\mathbb{Z}_a \times \mathbb{Z}_b$ for any a and b positive integers.

(ii) Algorithms for distance based topological indices for complete m-ary trees for $m > 3$ and for different heights H.

6.2 Future Work

(i) Construction algorithm and algorithm for eccentric topological indices for zero divisor graphs containing commutative rings $\mathbb{Z}_n$.

(ii) Degree Based topological indices for zero divisor graph.

(iii) Edge eccentric topological indices for two dimensional conductive metallic organic framework $Cu_3(HITP)_2[m.n]$.

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