Computing Connection Number-Based Indices for Graphs Derived from Metal Organic

By

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CIIT/FA21-RMT-068/LHR

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Declaration

I Muhammad Adeel Arshad with registration number CIIT/FA21-RMT-068/LHR hereby declares that I have produced the work presented in this report, during the scheduled period of study. I also declare that I have not taken any material from any source except referred to wherever due, that the amount of plagiarism is within acceptable range. If a violation of HEC rules on research has occurred in this thesis, I shall be liable to punishable action under the plagiarism rules of the HEC.

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It is certified that **<u>Muhammad Adeel Arshad with registration number CIIT/FA21-RMT-068/LHR</u>** has carried out all the work related to this report under my supervision at the Department of Mathematics, COMSATS University Islamabad, Lahore Campus, and the work fulfills the requirement for award of MS degree.

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DEDICATION

To

To My Parents, My Family
And My All Teachers

ACKNOWLEDGEMENT

Praise to be ALLAH, the Cherisher and Lord of the World, Most gracious and Most Merciful

First and foremost, I would like to express my sincere gratitude to Allah Almighty, the most beneficent and merciful, for granting us the strength, knowledge, abilities, and opportunities to undertake this research study and see it through to completion. Without the countless blessings of Allah Almighty, this accomplishment would not have been possible. May His peace and blessings be upon His messenger, Hazrat Muhammad (PBUH), his family, companions, and all those who follow in his footsteps. We are eternally grateful to Hazrat Muhammad (PBUH), who serves as an eternal source of guidance and knowledge for all of humanity.

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ABSTRACT

Computing Connection Number-Based Indices for Graphs Derived from Metal Organic

Metal-organic networks consist of metals and organic ligands, forming their two distinctive components. In the realm of Mathematical Chemistry, metals are elements that exhibit metallic bonding and possess a propensity to readily form positive ions. Ligands, on the other hand, encompass neutral molecules or ions that attach to the central atoms or ions of metals, forming bonds. The recent surge in the significance of distance-based topological indices has led to their widespread use in exploring the structure-property relationship among molecules. Given their importance, this thesis focuses specifically on distance-based topological indices. It delves into Metal-organic Networks, examining their characteristics and properties. The thesis also involves the computation of several connection-based Zagreb indices to gain insights into the Metal-organic Networks. By emphasizing the role of distance-based topological indices, this study aims to contribute to our understanding of Metal-organic Networks and their structural features. The examination of these indices offers valuable information regarding connectivity and complexity, facilitating further research and potential applications in fields such as materials science, catalysis, and drug discovery.

.

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Chapter 1

Introduction

1.1 History

The Seven Bridges of Konigsberg problem first arise roughly 300 years ago, at a time when nobody was familiar with the field of graph theory. At the time, Konigsberg was a German city; today, it is a Russian city situated alongside the Pregel river.This city has seven bridges, and they were used to connect it to two islands. The residents of Königsberg have long wondered whether it is possible to cross all seven bridges without having to do it more than once. Leonhard Euler (1707-1783) was the person who had figured out the problem in 1736[17]. Euler's conclusion regarding the issue was that it was either impossible or impractical to cross the bridges in a single attempt except cross the other bridges more than one time. In order to mark the problem in a fairly straightforward manner, he used the dots to represent the landmasses as vertices and lines to represent the seven bridges as edges. He not only demonstrated that it is impossible, but he also provided the explanation for why this is the case.He simplify this by introducing the new term valence or degree of vertex as a count of edges connecting to a specific vertex. The Eulerian graph is the result of the Euler idea.Actually, this Eulerian idea created a brand-new branch of the mathematics called "Graph Theory".

After a century, Kirchhoff assemble still another advancement in that area when he was experimenting with electronic networks[7]. The characteristics of a brand-new class of graphs termed trees has been put out by Sylvester and Caley. A different area of mathematics called linear algebra and graph theory are closely related. Poincare made yet another discovery in the foundations of graph theory that is related to incidence matrix and matrix theory. Mobius made the discovery of the family's collection of complete graphs in 1840. The four color problem was created by Gutherie in the theory of graphs in 1852. Graph theory is a subject that is currently being utilized in many scientific domains, including computer science like networks, chemistry like chemical graphs, electronics like electronically circuits, operations research as drainage systems, traffics flow, and telephone lines. It is also utilized in optimization issues. Graph theory has several uses that are extremely beneficial to people. Although graph theory belongs to Mathematics, its roots can be found in many other fields including statistical data, Mechanical, Civil and Chemical Engineering.

1.2 Elements of Basic Graph Theory

In this section we discussed some basic definations of graph theory that is useful for understanding the chemical structures.

1.2.1 Graph

A graph $\mathbb{F}$ is made up of non-empty finite set V($\mathbb{F}$) of vertices (or nodes) and a non-empty finite set E($\mathbb{F}$) of different unordered pairs of vertices V($\mathbb{F}$) called edges.We refer E($\mathbb{F}$) as edge set and V($\mathbb{F}$) as vertex set.
V($\mathbb{F}$)=$\{v_1, v_2, v_3, v_4, v_5\}$, E($\mathbb{F}$)=$\{e_1, e_2, e_3, e_4, e_5, e_6, e_7, e_8\}$

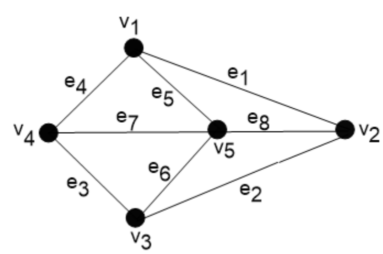

Figure 1.1: A graph $\mathbb{F}$

1.2.2 Subgraph

If a vertex set V($\mathbb{F}'$) and edge set E($\mathbb{F}'$) of $\mathbb{F}'$ are subsets of the vertex set V($\mathbb{F}'$) and edge set E($\mathbb{F}'$) of $\mathbb{F}$. Then we say that $\mathbb{F}'$ is a subgraph of $\mathbb{F}$.

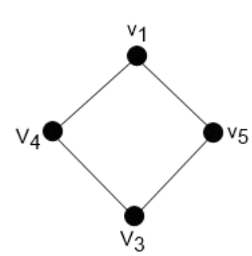

Figure 1.2: Subgraph($\mathbb{F}'$)

1.2.3 Size and Order of Graph

A graph's $|V|$ number of the vertices determines the order of graph.A graph's size is defined by its number of edges, or $|E|$.

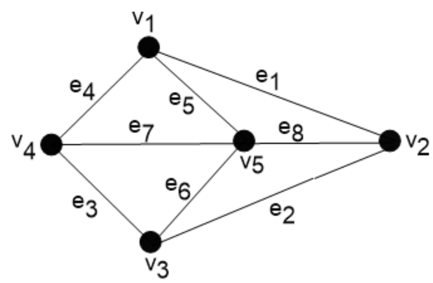

Figure 1.3: $|V(G)|$=5 and $|E(G)|$=8

1.2.4 Degree of Vertex

The amount of edges that are connected to a vertex is called the degree of that vertex in the graph.This is denoted by $d(v)$.

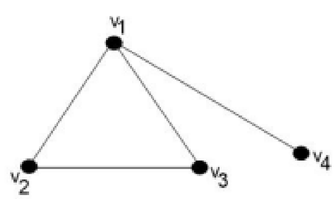

Figure 1.4: Vertices with degree

$d(v_1)$=3

$d(v_2)$=2

$d(v_3)$=2

$d(v_4)$=1

1.2.5 Isolated Vertex

A vertex is called an isolated vertex, if no edge is connected to that vertex.In other words, the vertex of 0 degree is called isolated vertex.

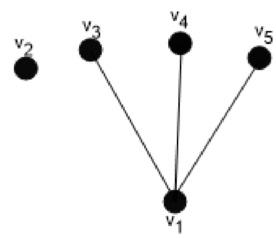

Figure 1.5: v_2 is an isolated vertex.

1.2.6 Pendant Vertex

A vertex of the degree 1 is called pendant vertex. In Figure 1.5 v_3, v_4, v_5 are pendant vertices.

1.2.7 Odd Vertex

A vertex is said to be an odd vertex, if number of edges connected to that vertex is odd. In other words, the vertex of odd degree is called an odd vertex.

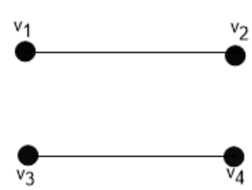

Figure 1.6: All the vertices are odd.

1.2.8 Even Vertex

A vertex is said to be an even vertex, if number of edges are connected to that vertex is even. In other words, the vertex of even degree is called even vertex.

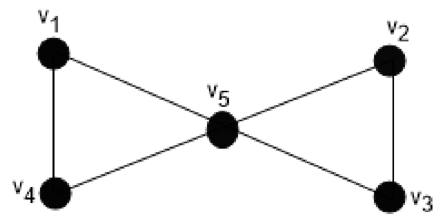

Figure 1.7: All the vertices are even.

1.2.9 Adjacent Vertices

If an edge connects two vertices in a graph, those vertices will be considered as adjacent.The single edge here that connects these two vertices keeps their vertices adjacent. In Fig 1.8,v_1 is adjacent to the v_2, v_3, except to v_4, v_5. Similarly, v_2 is only adjacent to the v_1, v_3, v_3 is adjacent to the v_1, v_2, v_4, v_4 is adjacent to v_3, v_5 and v_5 is only adjacent to the v_4.

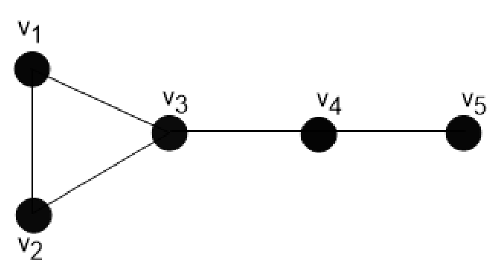

Figure 1.8: Graph with adjacent vertices.

1.2.10 Neighborhood Vertex Set

The neighbourhood vertex set ($N_{\mathbb{F}}(v)$) of every vertex v in a graph $\mathbb{F}$ consists of all the vertices adjacent to that vertex. Neighborhood of all vertices of Fig 1.1 are as follows:

$N_{\mathbb{F}}(v_1)$=$\{v_2, v_4, v_5\}$

$N_{\mathbb{F}}(v_2)$=$\{v_1, v_3, v_5\}$

$N_{\mathbb{F}}(v_3)$=$\{v_2, v_4, v_5\}$

$N_{\mathbb{F}}(v_4)$=$\{v_1, v_3, v_5\}$

$N_{\mathbb{F}}(v_5)$=$\{v_1, v_2, v_3, v_4\}$

1.2.11 Loop

When an edge which joins the vertex to itself is known as loop, e_7 is a loop in this graph.

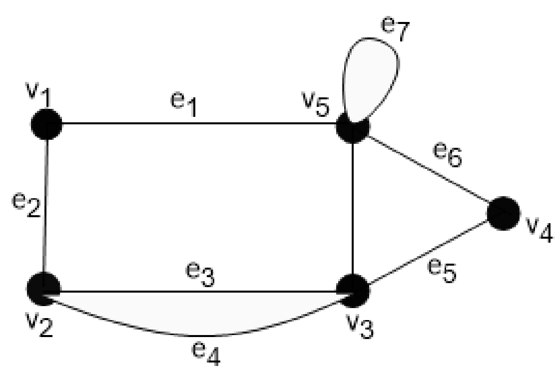

Figure 1.9: Graph with loop and multiple edges.

1.2.12 Multiple Edges

In a graph, multiple edges are any two or more than two edges these are connected to the same pair of two vertices.

In Fig 1.9, e_3 and e_4 are multiple edges.

1.2.13 Adjacent Edges

In a graph, two or more edges that are adjacent edges if these edges have the common vertex.

In Fig 1.10, e_3, e_4, e_2 are adjacent edges at v_2.

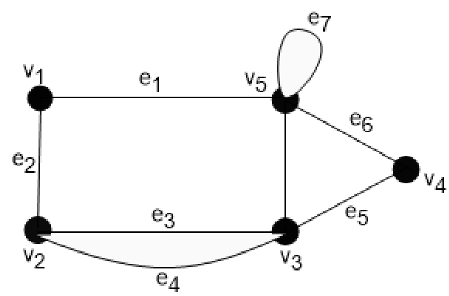

Figure 1.10: Graph with adjacent edges.

1.2.14 Pendent Edges

A graph $\mathbb{F}$'s edge will be considered a pendant edge when any one of its vertices is a pendant vertex.

In Fig 1.11 e_1 is the pendent edge.

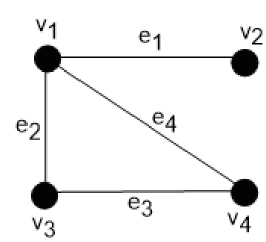

Figure 1.11: Graph with pendent edge.

1.2.15 Simple Graph

A simple graph is one that is unweighted, undirected, and free of loops or multiple edges. The graph in Fig 1.12 is simple graph.

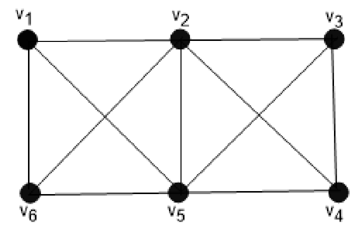

Figure 1.12: Graph with no loop and multiple edges.

1.2.16 Multiple Graph

If a graph $\mathbb{F}$'s has multiple edges or at least one loop, then its called multiple graph. The graph in Fig 1.13 is a multiple graph.

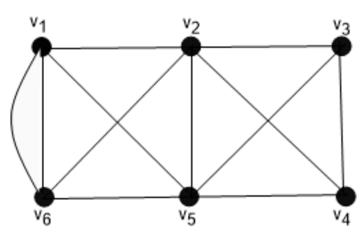

Figure 1.13: Graph with multiple edges.

1.2.17 Finite Graph

A graph is called finite if it has number of edges and vertices are finite.

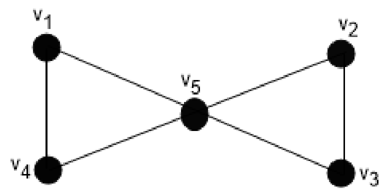

Figure 1.14: Finite graph

1.2.18 Infinite Graph

A graph is known as infinite if they have the number of edges and vertices are infinite.

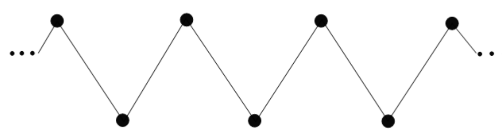

Figure 1.15: 2-Regular infinite graph

1.2.19 Planar Graph

If a graph is drawn on a plane aside from any edges are crossing, then it is said to be planar.

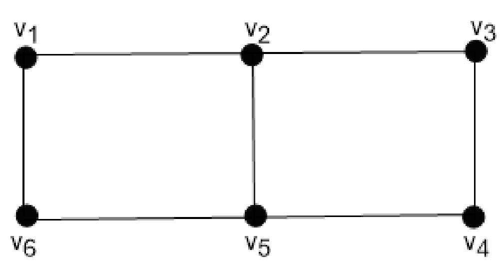

Figure 1.16: Planar graph

1.2.20 Non-Planar Graph

If a graph can be draw on a plane and if any two edges crossing each other, then it is said to be non-planar.

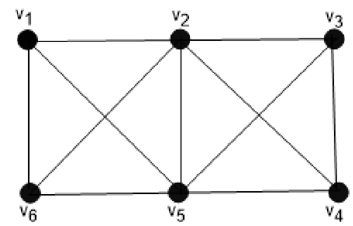

Figure 1.17: Non-planar graph

1.2.21 Regular Graph

If the degree of each vertex in the graph is equal, then this graph is said that regular.If each vertex's degree is K, a graph is said to be K regular..

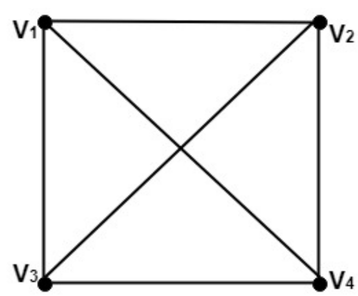

Figure 1.18: 3-Regular graph

1.2.22 Walk

A walk is a pattern of a graph's vertices and edges, therefore if we pass over the graph, we obtain a walk. In Fig 1.19 $v_1 -> v_5 -> v_6 -> v_2 -> v_3 -> v_4 -> v_3 -> v_2$ is a walk.

1.2.23 Path

A Path is like walk but no vertex and edge is repeated in this walk. In Fig 1.19 $v_1->v_2->v_3->v_4$ is a path.

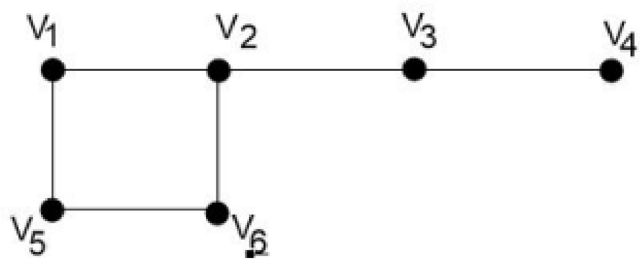

Figure 1.19: Graph with walk and path

1.2.24 Cyclic Graph

A graph that has at least one cycle, or a path that starts and end at the same vertex without going through any other vertices again, is referred to as cyclic graph. In Fig 1.20 $v_1->v_3->v_4->v_1$ is cycle.

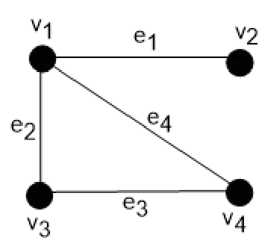

Figure 1.20: cyclic graph

1.2.25 Operation on Graphs

Take two graphs G_1=(V_1, E_1) and G_2=(V_2, E_2), then union of G_1 and G_2 is G=(V, E). Where V=$V_1 \cup V_2$,E=$E_1 \cup E_2$.

$$V(V_1 \cup V_2) = V(V_1) \cup V(V_2)$$

$$E(E_1 \cup E_2) = E(E_1) \cup (E_2)$$

.

$$V(V_1 \cap V_2) = V(V_1) \cap V(V_2)$$

$$E(E_1 \cap E_2) = E(E_1) \cap (E_2)$$

.

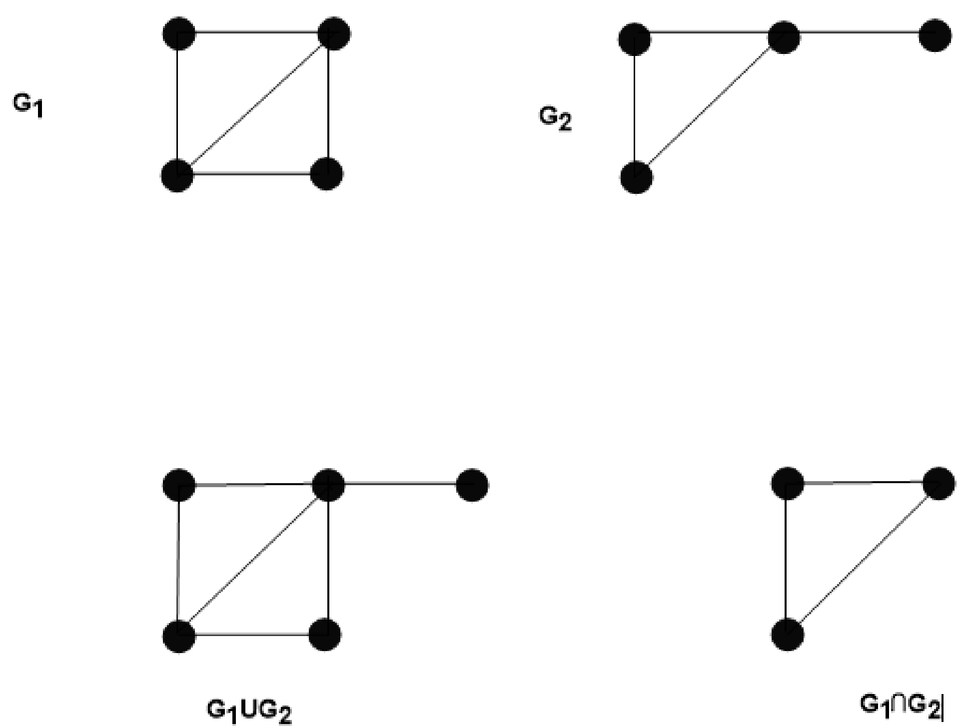

Figure 1.21: Operations on graph

Chapter 2

Literature Review

2.1 Introduction

A branch of mathematics called chemical graph theory that merge chemistry and graph theory. Chemical graph theory focuses on all aspects of applying graph theory to chemistry, including computational, theoretical, mathematical, and organic chemistry, as well as bioinformatics and chemoinformatics. Topological indices are mathematical invariants of chemical graphs, have shown to be useful tools for studying compounds' physio-chemical properties. In chemical graph theory, topological indices are especially important for the study of (QSPR/QSAR).

The topological index can be seen as a distance metric that employs each chemical structure's numerical value as a descriptor for the molecule under study. The Zagreb index,Weiner index, sum connectivity index is well known indices in graph theory. In 2021, we find the degree based topological indices of Supramolecular chain In dialkyltin complexes Of N-salicylidene-L-valine[1]. Degree-based topological indices, distance-based topological indices and spectrum-based topological indices are the three types of topological indices that are commonly used. Recently distance based topological indices gain great importance and use in the set of several different types of topological indices. They're often used to investigate the structure-property relationship between molecules. Because of the importance of distance-based topological indices in this thesis we will focus on the distance-based topological indices.

Recently, Naji et al. [16], has introduced the three connection based topological indices named as,

First Zagreb Connection Index.

Second Zagreb Connection Index.

Third Zagreb Connection Index.

2.2 Connection Number of Vertex

The connection number of a vertex v is defined as the number of the vertices at a distance two from that vertex v. It is denoted by $\overline{w}(v)$.

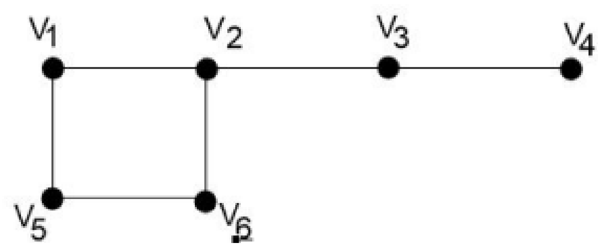

Figure 2.1: Connection number of v_1,v_2,v_3,v_6 is 2 and connection number of v_4,v_5 is 1.

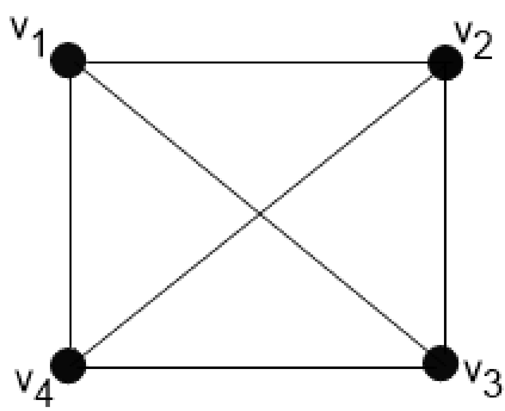

Figure 2.2: Connection number of all vertices is 3.

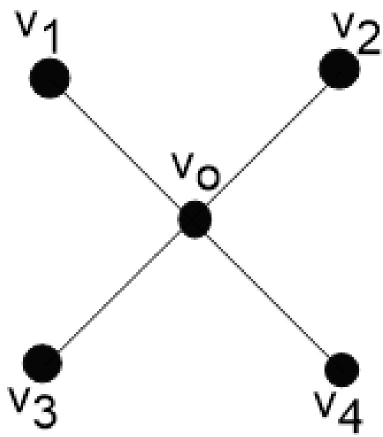

Figure 2.3: Connection number of v_o is 0 and connection number of all other vertices is 3.

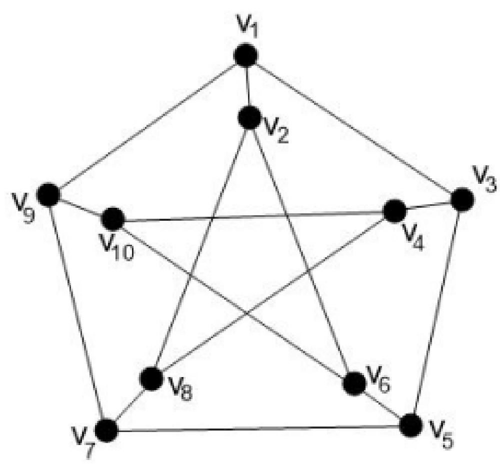

Figure 2.4: Connection number of all other vertices is 6.

2.3 Distance Based Topological Indices

Topological indices can be calculated using the concept of degree of vertices and/or distance between two vertices. In this thesis, we discussed the distance based topological indices.

One of the most famous and oldest topological index is Wiener Index W(G). Wiener index is defined as the sum of distances between any two atoms(vertices) in the molecules, in terms of bonds (or edges). This index introduced by chemist Harold Wiener[21] in 1947. In 1972, Gutman and Trinajsti ́c[13] defined the first degree-base topological index named as first Zagreb index(M1) to calculate the pi-energy of linked molecules. After that year, the 2nd Zagreb Index (M2) was created by Gutman et al[14]. Many scientists and mathematicians later used these topological indices thanks to theory and applications like operations on graphs[18, 8]. Furtula and Ivan Gutman[10] introduced the third Zagreb index(forgotten index) in 2015. Zagreb type indices have various applications in mathematical chemistry and computational graph theory that's why lot of researchers work on the Zagreb type indices[6, 15, 5].

Recently, first Zagreb connection index$(\hat{Z}C_1)$was introduced by Naji.[20] in 2017 and second Zagreb connection index $(\hat{Z}C_2)$ was introduced by Naji and Soner in 2018. Ali and Trinajstic[3] introduced modified first Zagreb connection index$(\hat{Z}C_1^*)$ in 2018. Similarly modified Zagreb connection indices and multiplicative modified Zagreb connection indices are recently introduced by Javaid[19]. We cite for further information on the characteristics and investigations of Zagreb connection indices[9, 4, 11, 12].

2.4 Zagreb Connection Index

First Zagreb connection index of graph($\mathbb{F}$) is:

$$\hat{Z}C_1(\mathbb{F}) = \sum_{v \in V(\mathbb{F})} [\overline{w}_{\mathbb{F}}(v)]^2, \tag{2.4.1}$$

and second Zagreb connection index of graph($\mathbb{F}$)is :

$$\hat{Z}C_2(\mathbb{F}) = \sum_{uv \in E(\mathbb{F})} [\overline{w}_{\mathbb{F}}(u) \times \overline{w}_{\mathbb{F}}(v)], \tag{2.4.2}$$

where $\overline{w}(u)$ represent connection number of u and $\overline{w}(v)$ represent the connection number of v to the edge uv.

2.5 Modified Zagreb Connection Indices(mZCI)

Modified Zagreb connection indices are:

$$ZC_1^*(\mathbb{F}) = \sum_{uv \in E(\mathbb{F})} [\overline{w}_{\mathbb{F}}(u) + \overline{w}_{\mathbb{F}}(v)] \tag{2.5.1}$$

$$\hat{Z}C_2^*(\mathbb{F}) = \sum_{uv \in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(v) + d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(u)] \tag{2.5.2}$$

$$\hat{Z}C_3^*(\mathbb{F}) = \sum_{uv \in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(u) + d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(v)] \tag{2.5.3}$$

$$\hat{Z}C_4^*(\mathbb{F}) = \sum_{uv \in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(u) \times d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(v)] \tag{2.5.4}$$

Where,

$\hat{Z}C_1^*(\mathbb{F})$ represent 1^{st} mZCI.

$\hat{Z}C_2^*(\mathbb{F})$ represent 2^{nd} mZCI.

$\hat{Z}C_3^*(\mathbb{F})$ represent 3^{rd} mZCI.

$\hat{Z}C_4^*(\mathbb{F})$ represent 4^{th} mZCI.

2.6 Multiplicative Zagreb Connection Indices(MZCI)

Multiplicative Zagreb connection indices are:

$$M\hat{Z}C_1(\mathbb{F}) = \prod_{v\in V(\mathbb{F})} [\overline{w}_{\mathbb{F}}(v)]^2 \tag{2.6.1}$$

$$M\hat{Z}C_2(\mathbb{F}) = \prod_{uv\in E(\mathbb{F})} [\overline{w}_{\mathbb{F}}(u) \times \overline{w}_{\mathbb{F}}(v)] \tag{2.6.2}$$

$$M\hat{Z}C_3(\mathbb{F}) = \prod_{uv\in E(\mathbb{F})} [d_{\mathbb{F}}(u) \times \overline{w}_{\mathbb{F}}(v)] \tag{2.6.3}$$

$$M\hat{Z}C_4(\mathbb{F}) = \prod_{uv\in E(\mathbb{F})} [\overline{w}_{\mathbb{F}}(u) + \overline{w}_{\mathbb{F}}(v)] \tag{2.6.4}$$

where,

$M\hat{Z}C_1(\mathbb{F})$ represent 1^{st} MZCI.

$M\hat{Z}C_2(\mathbb{F})$ represent 2^{st} MZCI.

$M\hat{Z}C_3(\mathbb{F})$ represent 3^{st} MZCI.

$M\hat{Z}C_4(\mathbb{F})$ represent 4^{st} MZCI.

2.7 Modified Multiplicative Zagreb Connection Indices(mMZCI)

Modified multiplicative Zagreb connection indices are:

$$M\hat{Z}C_1^*(\mathbb{F}) = \prod_{uv\in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(v) + d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(u)] \tag{2.7.1}$$

$$M\hat{Z}C_2^*(\mathbb{F}) = \prod_{uv\in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(u) + d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(v)] \tag{2.7.2}$$

$$M\hat{Z}C_3^*(\mathbb{F}) = \prod_{uv\in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(u) \times d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(v)] \tag{2.7.3}$$

Where,

$M\hat{Z}C_1^*(\mathbb{F})$ represent 1^{st} mMZCI.

$M\hat{Z}C_2^*(\mathbb{F})$ represent 2^{st} mMZCI.

$M\hat{Z}C_3^*(\mathbb{F})$ represent 3^{st} mMZCI.

Chapter 3

Metal-Organic Networks

In this chapter, we calculate the results for topological indices, which are based on degree of vertices and connection number of vertices in metal-organic networks. We compute Zagreb and modified Zagreb connection indices,multiplicative and modified multiplicative Zagreb connection indices of metal-organic networks.

3.1 First Metal-Organic Network($MON_1(p)$)

In this section, we review metal-organic networks [2]. Firstly we discuss basic metal-organic network which are made up of two different components metals and organic ligands.The smaller vertices are organic ligands, while the bigger vertices/atoms are metals,that are zeolite imidazole which is shown in Fig. (3.1). Moreover, the metal-organic network($M0N_1$(p)) is established by joining the metals of the two key layers of the fundamental metal-organic network in such a way that the outer layers two metals are connected to the inner layers metals. For $p \geq 2$, the $|V(MON_1(p))| = |V(MON_2(p))| = 48p$ and $|E(MON_1(p))| = |E(MON_2(p))| = 72p - 12p$. For $p = 2$ first metal-organic network is shown in Fig. (3.2).

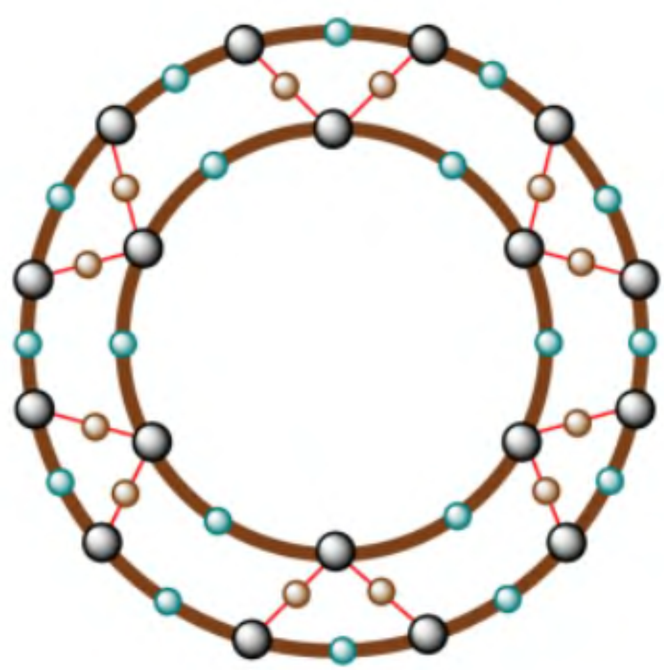

Figure 3.1: Basic metal-organic network($MON(p)$)

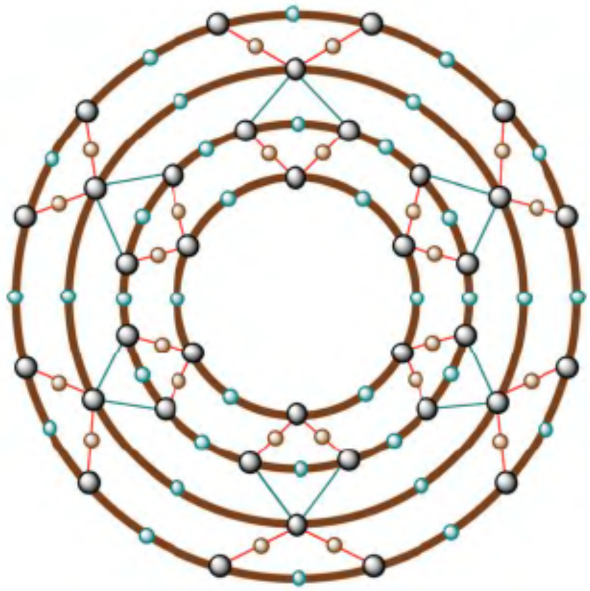

Figure 3.2: First metal-organic network($MON_1(p)$ for $p=2$)

$V_{\overline{w}(u)}$	$\lvert V_{\overline{w}(u)}\rvert$
V_3	12
V_4	18
V_5	$6p-6$
V_6	$6p+12$
V_7	$12p$
V_8	$12p-24$
V_9	$6p-6$
V_{10}	$6p-6$

Table 3.1: Vertex partition of $MON_1(p)$ on the basis of vertex connection number

$E_{\overline{w}(u),\overline{w}(v)}$	$\lvert E_{\overline{w}(u),\overline{w}(v)}\rvert$
$E_{3,4}$	24
$E_{3,7}$	12
$E_{4,6}$	24
$E_{5,7}$	$12p-12$
$E_{6,7}$	$12p$
$E_{7,8}$	$12p-24$
$E_{7,9}$	$12p$
$E_{8,9}$	$12p-24$
$E_{9,10}$	$12p-12$

Table 3.2: Edge partition of $MON_1(p)$ on the basis of connection number

$E_{d(u),d(v)}^{\overline{w}(u),\overline{w}(v)}$	$\lvert E_{d(u),d(v)}^{\overline{w}(u),\overline{w}(v)}\rvert$
$E_{3,2}^{3,4}$	24
$E_{3,2}^{3,7}$	12
$E_{4,2}^{4,6}$	24
$E_{2,4}^{5,7}$	$12p-12$
$E_{2,4}^{6,7}$	$12p$
$E_{4,2}^{7,8}$	$12p-24$
$E_{2,6}^{7,9}$	12
$E_{4,6}^{7,9}$	$12p-12$
$E_{2,6}^{8,9}$	$12p-24$
$E_{6,2}^{9,10}$	$12p-12$

Table 3.3: Edge partition of $MON_1(p)$ on the basis of degree-connection number

3.2 Main result of $MON_1(p)$

Theorem 3.2.1. *For the first metal organic network $\mathbb{F} \approxeq MON_1(p)$, the first Zagreb connection index $\hat{Z}C_1(\mathbb{F})$ is,*

$$\hat{Z}C_1(\mathbb{F}) = 2808p - 1944.$$

Proof. By using Defination 2.4.1:

$$\hat{Z}C_1(\mathbb{F}) = \sum_{v \in V(\mathbb{F})} [\overline{w}_{\mathbb{F}}(v)]^2.$$

By using Table:3.1

$$\hat{Z}C_1(\mathbb{F}) = (3)^2(12) + (4)^2(18) + (5)^2(6p-6) + (6)^2(6p+12) + (7)^2(12p) + (8)^2(12p-24) + (9)^2(6p-6) + (10)^2(6p-6)$$

After solving it, we get our result:

$$= 2808p - 1944.$$

□

Theorem 3.2.2. *For the first metal organic network $\mathbb{F} \approxeq MON_1(p)$, the second Zagreb connection index $\hat{Z}C_2(\mathbb{F})$ is,*

$$\hat{Z}C_2(\mathbb{F}) = 4296p - 3456.$$

Proof. By using Defination 2.4.2:

$$\hat{Z}C_2(\mathbb{F}) = \sum_{uv \in E(\mathbb{F})} [\overline{w}_{\mathbb{F}}(u) \times \overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.2

$$\hat{Z}C_2(\mathbb{F}) = (3 \times 4)(24) + (3 \times 7)(12) + (4 \times 6)(24) + (5 \times 7)(12p-12) + (6 \times 7)(12p) + (7 \times 8)(12p-24) + (7 \times 9)(12p) + (8 \times 9)(12p-24) + (9 \times 10)(12p-12)$$

After solving it, we get our result:

$$= 4296p - 3456.$$

□

Theorem 3.2.3. *For the first metal organic network $\mathbb{F} \approxeq MON_1(p)$, the modified first Zagreb connection index $\hat{Z}C_1^*(\mathbb{F})$ is,*

$$\hat{Z}C_1^*(\mathbb{F}) = 1104p - 612.$$

Proof. By using Defination 2.5.1:

$$\hat{Z}C_1^*(\mathbb{F}) = \sum_{uv \in E(\mathbb{F})} [\overline{w}_{\mathbb{F}}(u) + \overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.2

$$\begin{aligned}\hat{Z}C_1^*(\mathbb{F}) =&(3+4)(24)+(3+7)(12)+(4+6)(24)+(5+7)(12p-12)+(6+7)(12p)+\\ &(7+8)(12p-24)+(7+9)(12p)+(8+9)(12p-24)+(9+10)(12p-12)\end{aligned}$$

After solving it, we get our result:

$$= 1104p - 612.$$

□

Theorem 3.2.4. *For the first metal organic network $\mathbb{F} \approxeq MON_1(p)$, the modified second Zagreb connection index $\hat{Z}C_2^*(\mathbb{F})$ is,*

$$\hat{Z}C_2^*(\mathbb{F}) = 4080p - 3120.$$

Proof. By using the Defination 2.5.2;

$$\hat{Z}C_2^*(\mathbb{F}) = \sum_{uv \in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(v) + d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(u)].$$

By using Table:3.2

$$\begin{aligned}\hat{Z}C_2^*(\mathbb{F}) =&((3)(4)+(2)(3))(24)+((3)(7)+(2)(3))(12)+((4)(6)+(2)(4))(24)+\\ &((12)(7)+(4)(5))(12p-12)+((2)(7)+(4)(6))(12p)+((4)(8)+(2)(7))(12p-24)+\\ &((2)(9)+(6)(7))(12)+((4)(9)+(6)(7))(12p-12)+((2)(9)+(6)(8))(12p-24)+\\ &((6)(10)+(2)(9))(12p-1)\end{aligned}$$

After solving it, we get our result:

$$= 4080p - 3120.$$

$\square$

Theorem 3.2.5. *For the first metal organic network $\mathbb{F} \approxeq MON_1(p)$, the modified third Zagreb connection index $\hat{Z}C_3^*(\mathbb{F})$ is,*

$$\hat{Z}C_3^*(\mathbb{F}) = 4176p - 2892.$$

Proof. By using the Defination 2.5.3;

$$\hat{Z}C_3^*(\mathbb{F}) = \sum_{uv \in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(u) + d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.3

$$\begin{aligned}\hat{Z}C_3^*(\mathbb{F}) =& ((3)(3)+(2)(4))(24)+((3)(3)+(2)(7))(12)+((4)(4)+(2)(6))(24)+\\ &((2)(5)+(4)(7))(12p-12)+((2)(6)+(4)(7))(12p)+((4)(7)+(2)(8))(12p-24)+\\ &((2)(7)+(6)(9))(12)+((4)(7)+(6)(9))(12p-12)+((2)(8)+(6)(9))(12p-24)+\\ &((6)(9)+(2)(10))(12p-12)\end{aligned}$$

After solving it, we get our result:

$$= 4176p - 2892.$$

$\square$

Theorem 3.2.6. *For the first metal organic network $\mathbb{F} \approxeq MON_1(p)$, the modified fourth Zagreb connection index $\hat{Z}C_4^*(\mathbb{F})$ is,*

$$\hat{Z}C_4^*(\mathbb{F}) = 54240p - 49032.$$

Proof. By using Defination 2.5.4:

$$\hat{Z}C_4^*(\mathbb{F}) = \sum_{uv\in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(u) \times d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.3

$$\begin{aligned}\hat{Z}C_4^*(\mathbb{F}) =&((3)(3)\times(2)(4))(24)+((3)(3)\times(2)(7))(12)+((4)(4)\times(2)(6))(24)+\\&((2)(5)\times(4)(7))(12p-12)+((2)(6)\times(4)(7))(12p)+((4)(7)\times(2)(8))(12p-24)+\\&((2)(7)\times(6)(9))(12)+((4)(7)\times(6)(9))(12p-12)+((2)(8)\times(6)(9))(12p-24)+\\&((6)(9)\times(2)(10))(12p-12)\end{aligned}$$

After solving it, we get our result:

$$= 54240p - 49032.$$

□

Theorem 3.2.7. *For the first metal organic network $\mathbb{F} \approxeq MON_1(p)$, the first multiplicative Zagreb connection index $M\hat{Z}C_1(\mathbb{F})$ is,*
$M\hat{Z}C_1(\mathbb{F}) = 132705010046730240000p^6 - 398115030140190720000p^5 - 132705010046730240000p^4 + 1.4597551105140326e+21p^3 - 1.592460120560763e+21p^2 + 530820040186920960000p.$

Proof. By using Defination 2.6.1:

$$\hat{Z}C_1(\mathbb{F}) = \prod_{v\in V(\mathbb{F})} [\overline{w}_{\mathbb{F}}(v)]^2.$$

By using Table:3.1

$$\begin{aligned}M\hat{Z}C_1(\mathbb{F}) =&(3)^2(12)\times(4)^2(18)\times(5)^2(6p-6)\times(6)^2(6p+12)\times(7)^2(12p)\times(8)^2(12p-24)\times\\&(9)^2(6p-6)\times(10)^2(6p-6)\end{aligned}$$

After solving it, we get our result:

$$=13270501004673024000 0p^6 - 39811503014019072000 0p^5 - 13270501004673024000 0p^4 + 1.4597551105140326e + 21p^3 - 1.592460120560763e + 21p^2 + 53082004018692096000 0p.$$

$\square$

Theorem 3.2.8. *For the first metal organic network $\mathbb{F} \approxeq MON_1(p)$, the second multiplicative Zagreb connection index $M\hat{Z}C_2(\mathbb{F})$ is,*
$M\hat{Z}C_2(\mathbb{F}) = 4.194922147985984e + 24p^5 - 2.5169532887915904e + 25p^4 + 5.453398792381779e + 25p^3 - 1.033906577583181e + 25p^2 + 1.6779688591943936e + 25p.$

Proof. By using the Defination 2.6.2;

$$M\hat{Z}C_2(\mathbb{F}) = \prod_{uv \in E(\mathbb{F})} [\overline{w}_{\mathbb{F}}(u) \times \overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.2

$$M\hat{Z}C_2(\mathbb{F}) = (3 \times 4)(24) \times (3 \times 7)(12) \times (4 \times 6)(24) \times (5 \times 7)(12p - 12) \times (6 \times 7)(12p) \times (7 \times 8)(12p - 24) \times (7 \times 9)(12p) \times (8 \times 9)(12p - 24) \times (9 \times 10)(12p - 12)$$

After solving it, we get our result:

$$=4.194922147985984e + 24p^5 - 2.5169532887915904e + 25p^4 + 5.453398792381779e + 25p^3 - 1.033906577583181e + 25p^2 + 1.6779688591943936e + 25p.$$

$\square$

Theorem 3.2.9. *For the first metal organic network $\mathbb{F} \approxeq MON_1(p)$,nthe third multiplicative Zagreb connection index $M\hat{Z}C_3(\mathbb{F}$ is,*
$M\hat{Z}C_3(\mathbb{F}) = 6.57489838704742e + 24p^6 - 4.602428870933194e + 25p^5 + 1.2492306935390098e + 26p^4 - 1.643724596761855e + 26p^3 + 1.0519837419275872e + 26p^2 - 2.629959354818968e + 25p.$

Proof. By using Defination 2.6.3:

$$M\hat{Z}C_3(\mathbb{F}) = \prod_{uv \in E(\mathbb{F})} [d_{\mathbb{F}}(u) \times \overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.3

$$\begin{aligned} M\hat{Z}C_3(\mathbb{F}) =& (3\times 4)(24) \times (3\times 7)(12) \times (4\times 6)(24) \times (2\times 7)(12p-12) \times (2\times 7)(12p) \times \\ & (4\times 8)(12p-24) \times (2\times 9)(12) \times (4\times 9)(12p-12) \times (2\times 9)(12p-24) \times \\ & (6\times 10)(12p-12) \end{aligned}$$

After solving it, we get our result:

$$\begin{aligned} =& 6.57489838704742e+24p^6 - 4.602428870933194e+25p^5 + 1.2492306935390098e+26p^4 - \\ & 1.643724596761855e+26p^3 + 1.0519837419275872e+26p^2 - 2.629959354818968e+25p. \end{aligned}$$

$\square$

Theorem 3.2.10. *For the first metal organic network $\mathbb{F} \approxeq MON_1(p)$, the fourth multiplicative Zagreb connection index $M\hat{Z}C_4(\mathbb{F}$ is,*
$M\hat{Z}C_4(\mathbb{F}) = 174713960317059072000p^6 - 1.0482837619023544e+21p^5 + 2.271281484121768e+21p^4 - 2.0965675238047089e+21p^3 + 698855841268236288000p^2.$

Proof. By using Defination 2.6.4:

$$M\hat{Z}C_4(\mathbb{F}) = \prod_{uv \in E(\mathbb{F})} [\overline{w}_{\mathbb{F}}(u) + \overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.2

$$\begin{aligned} M\hat{Z}C_4(\mathbb{F}) =& (3+4)(24) \times (3+7)(12) \times (4+6)(24) \times (5+7)(12p-12) \times (6+7)(12p) \times \\ & (7+8)(12p-24) \times (7+9)(12p) \times (8+9)(12p-24) \times (9+10)(12p-12) \end{aligned}$$

After solving it, we get our result:

$$=17471396031705907200 0p^6 - 1.0482837619023544e + 21p^5 + 2.271281484121768e + 21p^4 - 2.0965675238047089e + 21p^3 + 698855841268236288000p^2.$$

□

Theorem 3.2.11. *For the first metal organic network $\mathbb{F} \approxeq MON_1(p)$, the modified first multiplicative Zagreb connection index $M\hat{Z}C_1^*(\mathbb{F})$ is,*
$M\hat{Z}C_1^*(\mathbb{F}) = 5.515227556984977e+27p^6 - 3.8606592898894836e+28p^5 + 1.0478932358271454e+29p^4 - 1.3788068892462441e+29p^3 + 8.824364091175963e+28p^2 - 2.2060910227939907e+28p.$

Proof. By using Defination 2.7.1:

$$M\hat{Z}C_1^*(\mathbb{F}) = \prod_{uv \in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(v) + d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(u)].$$

By using Table:3.3

$$\begin{aligned} M\hat{Z}C_1^*(\mathbb{F}) =& ((3)(4)+(2)(3))(24) \times ((3)(7)+(2)(3))(12) \times ((4)(6)+(2)(4))(24)\times \\ & ((12)(7)+(4)(5))(12p-12) \times ((2)(7)+(4)(6))(12p) \times ((4)(8)+(2)(7))(12p-24)\times \\ & ((2)(9)+(6)(7))(12) \times ((4)(9)+(6)(7))(12p-12) \times ((2)(9)+(6)(8))(12p-24)\times \\ & ((6)(10)+(2)(9))(12p-12) \end{aligned}$$

After solving it, we get our result:

$$=5.515227556984977e+27p^6 - 3.8606592898894836e+28p^5 + 1.0478932358271454e+29p^4 - 1.3788068892462441e+29p^3 + 8.824364091175963e+28p^2 - 2.2060910227939907e+28p.$$

□

Theorem 3.2.12. *For the first metal organic network $\mathbb{F} \approxeq MON_1(p)$, the modified second multiplicative Zagreb connection index $M\hat{Z}C_2^*(\mathbb{F})$ is,*

$M\hat{Z}C_2^*(\mathbb{F}) = 5.2378858531144462e+27p^6 - 3.666520097180123e+28p^5 +$
$9.951983120917477e+28p^4 - 1.3094714632786155e+29p^3 + 8.380617364983138e+$
$28p^2 - 2.0951543412457846e+28p.$

Proof. By using the Defination 2.7.2;

$$M\hat{Z}C_2^*(\mathbb{F}) = \prod_{uv \in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(u) + d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.3

$$\begin{aligned} M\hat{Z}C_2^*(\mathbb{F}) =&((3)(3)+(2)(4))(24) \times ((3)(3)+(2)(7))(12) \times ((4)(4)+(2)(6))(24) \times \\ &((2)(5)+(4)(7))(12p-12) \times ((2)(6)+(4)(7))(12p) \times ((4)(7)+(2)(8))(12p-24) \times \\ &((2)(7)+(6)(9))(12) \times ((4)(7)+(6)(9))(12p-12) \times ((2)(8)+(6)(9))(12p-24) \times \\ &((6)(9)+(2)(10))(12p-12) \end{aligned}$$

After solving it, we get our result:

$$\begin{aligned} =&5.2378858531144462e+27p^6 - 3.666520097180123e+28p^5 + 9.951983120917477e+28p^4 - \\ &1.3094714632786155e+29p^3 + 8.380617364983138e+28p^2 - 2.0951543412457846e+28p. \end{aligned}$$

□

Theorem 3.2.13. *For the first metal organic network $\mathbb{F} \approxeq MON_1(p)$, the modified third multiplicative Zagreb connection index $M\hat{Z}C_3^*(\mathbb{F})$ is,*
$M\hat{Z}C_3^*(\mathbb{F}) = 1.9393809682103555e+37p^6 - 1.357566677747249e+$
$38p^5 + 3.684823839599675e+38p^4 - 4.848452420525888e+38p^3 + 3.1030095491365685e+$
$38p^2 - 7.757523872841422e+37p.$

Proof. By using Defination 2.7.3:

$$M\hat{Z}C_3^*(\mathbb{F}) = \prod_{uv \in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(u) \times d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.3

$$\begin{aligned}M\hat{Z}C_3^*(\mathbb{F}) =&((3)(3)\times(2)(4))(24)\times((3)(3)\times(2)(7))(12)\times((4)(4)\times(2)(6))(24)\times\\&((2)(5)\times(4)(7))(12p-12)\times((2)(6)\times(4)(7))(12p)\times((4)(7)\times(2)(8))(12p-24)\times\\&((2)(7)\times(6)(9))(12)\times((4)(7)\times(6)(9))(12p-12)\times((2)(8)\times(6)(9))(12p-24)\times\\&((6)(9)\times(2)(10))(12p-12)\end{aligned}$$

After solving it, we get our result:

$$\begin{aligned}=&1.9393809682103555e+37p^6-1.357566677747249e+38p^5+3.684823839599675e+38p^4-\\&4.848452420525888e+38p^3+3.1030095491365685e+38p^2-7.757523872841422e+37p.\end{aligned}$$

$\square$

3.3 Second Metal-Organic Network($MON_2(p)$)

In this section, we discussed the formation of second metal organic-network($MON_2(p)$). In section 3.1 we discussed about the basic metal organic network.Now second metal-organic network($M0N_2(p)$) is established by the bonding of the organic ligands of two fundamental metal-organic networks, in which the organic ligands of two layers above one fundamental metal-organic network are connected with those of two layers below the second fundamental metal-organic network. For $p = 2$ second metal-organic network is shown in Fig. (3.4).

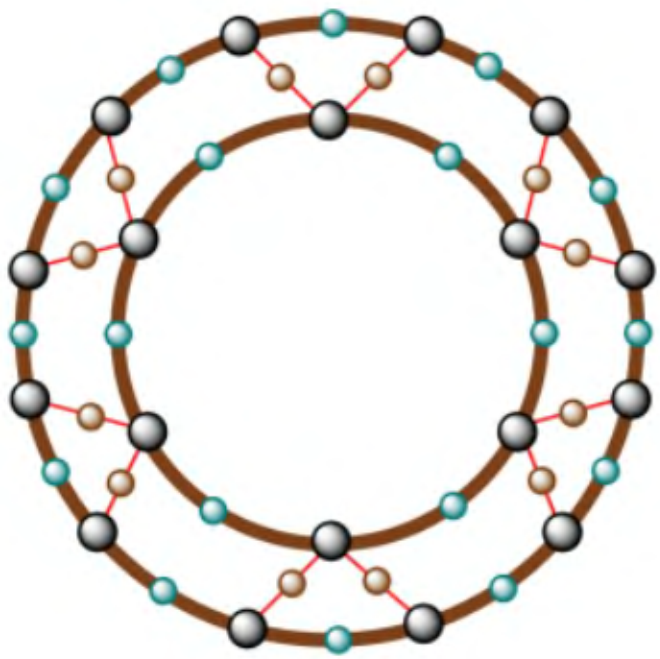

Figure 3.3: Basic metal-organic network($MON(p)$)

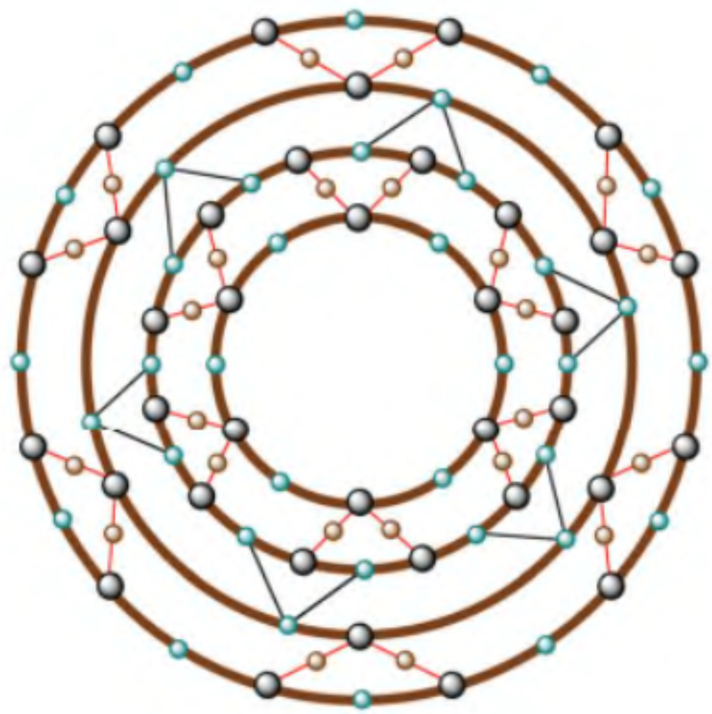

Figure 3.4: Second metal-organic network($MON_2(p)$ for $p = 2$)

$V_{\overline{w}(u)}$	$\lvert V_{\overline{w}(u)}\rvert$
V_3	12
V_4	$6p+12$
V_5	$18p-6$
V_6	$6p-12$
V_8	$6p-6$
V_9	$6p-6$

Table 3.4: Vertex partition of $MON_2(p)$ on the basis of vertex connection number

$E_{\overline{w}(u),\overline{w}(v)}$	$\lvert E_{\overline{w}(u),\overline{w}(v)}\rvert$
$E_{3,4}$	24
$E_{3,7}$	12
$E_{4,5}$	$6p+6$
$E_{4,6}$	$12p$
$E_{5,5}$	$6p-6$
$E_{5,6}$	$12p-12$
$E_{5,8}$	$12p-12$
$E_{6,9}$	$12p-12$
$E_{8,9}$	$12p-12$

Table 3.5: Edge partition of $MON_2(p)$ on the basis of connection number

$E_{d(u),d(v)}^{\overline{w}(u),\overline{w}(v)}$	$\lvert E_{d(u),d(v)}^{\overline{w}(u),\overline{w}(v)}\rvert$
$E_{3,2}^{3,4}$	24
$E_{3,2}^{3,5}$	12
$E_{3,2}^{4,5}$	$6p-6$
$E_{4,2}^{4,5}$	12
$E_{3,3}^{4,6}$	$12p-12$
$E_{4,2}^{4,6}$	12
$E_{2,3}^{5,5}$	$6p-6$
$E_{3,3}^{5,6}$	$12p-12$
$E_{2,4}^{5,8}$	$12p-12$
$E_{3,4}^{6,9}$	$12p-12$
$E_{4,4}^{8,9}$	$12p-12$

Table 3.6: Edge partition of $MON_2(p)$ on the basis of degree-connection number

3.4 Main result of $MON_2(p)$

Theorem 3.4.1. *For the second metal organic network $\mathbb{F} \approxeq MON_2(p)$, the first Zagreb connection index $\hat{Z}C_1(\mathbb{F})$ is,*

$$\hat{Z}C_1(\mathbb{F}) = 1848p - 936.$$

Proof. By using Defination 2.4.1:

$$\hat{Z}C_1(\mathbb{F}) = \sum_{v \in V(\mathbb{F})} [\overline{w}_{\mathbb{F}}(v)]^2.$$

By using Table:3.4

$$\hat{Z}C_1(\mathbb{F}) =(3)^2(12)+(4)^2(6p+12)+(5)^2(18p-6)+(6)^2(12p-6)+(8)^2(6p-6)+(9)^2(6p-6)$$

After solving it, we get our result:

$$= 1848p-936.$$

□

Theorem 3.4.2. *For the second metal organic network $\mathbb{F} \approxeq MON_2(p)$, the second Zagreb connection index $\hat{Z}C_2(\mathbb{F})$ is,*

$$\hat{Z}C_2(\mathbb{F}) = 2910p-1914.$$

Proof. By using Defination 2.4.2:

$$\hat{Z}C_2(\mathbb{F}) = \sum_{uv\in E(\mathbb{F})} [\overline{w}_{\mathbb{F}}(u) \times \overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.5

$$\begin{aligned}\hat{Z}C_2(\mathbb{F}) =&(3\times 4)(24)+(3\times 5)(12)+(4\times 5)(6p+6)+(4\times 6)(12p)+(5\times 5)(6p-6)+\\ &(5\times 6)(12p-12)+(5\times 8)(12p-12)+(6\times 9)(12p-12)+(8\times 9)(12p-12)\end{aligned}$$

After solving it, we get our result:

$$= 2910p-1914.$$

□

Theorem 3.4.3. *For the second metal organic network $\mathbb{F} \approxeq MON_2(p)$, the modified first Zagreb connection index $\hat{Z}C_1^*(\mathbb{F})$ is,*

$$\hat{Z}C_1^*(\mathbb{F}) = 906p-414.$$

Proof. By using Defination 2.5.1:

$$\hat{Z}C_1^*(\mathbb{F}) = \sum_{uv \in E(\mathbb{F})} [\overline{w}_{\mathbb{F}}(u) + \overline{w}_{\mathbb{F}}(u)].$$

By using Table:3.5

$$\hat{Z}C_1^*(\mathbb{F}) = (3+4)(24) + (3+5)(12) + (4+5)(6p+6) + (4+6)(12p) + (5+5)(6p-6) + (5+6)(12p-12) + (5+8)(12p-12) + (6+9)(12p-12) + (8+9)(12p-12)$$

After solving it, we get our result:

$$= 906p - 414.$$

□

Theorem 3.4.4. *For the second metal organic network $\mathbb{F} \approxeq MON_2(p)$, the modified second Zagreb connection index $\hat{Z}C_2^*(\mathbb{F})$ is,*

$$\hat{Z}C_2^*(\mathbb{F}) = 2904p - 1500.$$

Proof. By using the Defination 2.5.2;

$$\hat{Z}C_2^*(\mathbb{F}) = \sum_{uv \in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(v) + d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(u)].$$

By using Table:3.6

$$\hat{Z}C_2^*(\mathbb{F}) = ((3)(4)+(2)(3))(24) + ((3)(5)+(2)(3))(12) + ((3)(5)+(2)(4))(6p-6) + ((4)(5)+(2)(4))(12) + ((3)(6)+(3)(4))(12p-12) + ((4)(6)+(2)(4))(12) + ((2)(5)+(3)(5))(6p-6) + ((3)(6)+(3)(5))(12p-12) + ((2)(8)+(4)(5))(12p-12) + ((3)(9)+(4)(6))(12p-12) + ((4)(9)+(4)(8))(12p-12)$$

After solving it, we get our result:

$$= 2904p - 1500.$$

□

Theorem 3.4.5. *For the second metal organic network $\mathbb{F} \approxeq MON_2(p)$, the modified third Zagreb connection index $\hat{Z}C_3^*(\mathbb{F})$ is,*

$$\hat{Z}C_3^*(\mathbb{F}) = 3006p - 1722.$$

Proof. By using Defination 2.5.3:

$$\hat{Z}C_3^*(\mathbb{F}) = \sum_{uv \in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(u) + d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.6

$$\begin{aligned}\hat{Z}C_3^*(\mathbb{F}) =& ((3)(3)+(2)(4))(24) + ((3)(3)+(2)(5))(12) + ((3)(4)+(2)(5))(6p-6) + \\ & ((4)(4)+(2)(5))(12) + ((3)(4)+(3)(6))(12p-12) + ((4)(4)+(2)(6))(12) + \\ & ((2)(5)+(3)(5))(6p-6) + ((3)(5)+(3)(6))(12p-12) + ((2)(5)+(4)(8))(12p-12) + \\ & ((3)(6)+(4)(9))(12p-12) + ((4)(8)+(4)(9))(12p-12)\end{aligned}$$

After solving it, we get our result:

$$= 3006p - 1722.$$

□

Theorem 3.4.6. *For the second metal organic network $\mathbb{F} \approxeq MON_2(p)$, the modified fourth Zagreb connection index $\hat{Z}C_4^*(\mathbb{F})$ is,*

$$\hat{Z}C_4^*(\mathbb{F}) = 32892p - 26580.$$

Proof. By using Defination 2.5.4:

$$\hat{Z}C_4^*(\mathbb{F}) = \sum_{uv\in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(u) \times d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.6

$$\begin{aligned}\hat{Z}C_4^*(\mathbb{F}) =& ((3)(3)\times(2)(4))(24)+((3)(3)\times(2)(5))(12)+((3)(4)\times(2)(5))(6p-6)+\\ & ((4)(4)\times(2)(5))(12)+((3)(4)\times(3)(6))(12p-12)+((4)(4)\times(2)(6))(12)+\\ & ((2)(5)\times(3)(5))(6p-6)+((3)(5)\times(3)(6))(12p-12)+((2)(5)\times(4)(8))(12p-12)+\\ & ((3)(6)\times(4)(9))(12p-12)+((4)(8)\times(4)(9))(12p-12)\end{aligned}$$

After solving it, we get our result:

$$= 32892p - 26580.$$

□

Theorem 3.4.7. *For the second metal organic network $\mathbb{F} \approxeq MON_2(p)$, the first multiplicative Zagreb connection index $M\hat{Z}C_1(\mathbb{F})$ is,*
$M\hat{Z}C_1(\mathbb{F}) = 376147987660800p^5 - 313456656384000p^4 - 1065752631705600p^3 + 1692665944473600p^2 - 814987306598400p + 125382662553600.$

Proof. By using Defination 2.6.1:

$$\hat{Z}C_1(\mathbb{F}) = \prod_{v\in V(\mathbb{F})} [\overline{w}_{\mathbb{F}}(v)]^2.$$

By using Table:3.4

$$\begin{aligned}M\hat{Z}C_1(\mathbb{F}) =& (3)^2(12)\times(4)^2(6p+12)\times(5)^2(18p-6)\times(6)^2(12p-6)\times(8)^2(6p-6)\times\\ & (9)^2(6p-6)\end{aligned}$$

After solving it, we get our result:

$$=376147987660800p^5-313456656384000p^4-1065752631705600p^3+1692665944473600p^2-814987306598400p+125382662553600.$$

$\square$

Theorem 3.4.8. *For the second metal organic network $\mathbb{F}\approxeq MON_2(p)$, the second multiplicative Zagreb connection index $M\hat{Z}C_2(\mathbb{F})$is,*
$M\hat{Z}C_2(\mathbb{F}) = 2.5999348907114496e{+}22p^7 - 1.0399739562845798e{+}23p^6 + 1.2999674453557248e{+}23p^5 - 1.2999674453557248e{+}23p^3 + 1.0399739562845798e{+}23p^2 - 2.5999348907114496e{+}22p.$

Proof. By using the Defination 2.6.2;

$$M\hat{Z}C_2(\mathbb{F}) = \prod_{uv\in E(\mathbb{F})} [\overline{w}_{\mathbb{F}}(u)\times\overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.5

$$M\hat{Z}C_2(\mathbb{F}) =(3\times4)(24)\times(3\times5)(12)\times(4\times5)(6p+6)\times(4\times6)(12p)\times(5\times5)(6p-6)\times(5\times6)(12p-12)\times(5\times8)(12p-12)\times(6\times9)(12p-12)\times(8\times9)(12p-12)$$

After solving it, we get our result:

$$=2.5999348907114496e+22p^7-1.0399739562845798e+23p^6+1.2999674453557248e+23p^5-1.2999674453557248e+23p^3+1.0399739562845798e+23p^2-2.5999348907114496e+22p.$$

$\square$

Theorem 3.4.9. *For the second metal organic network $\mathbb{F}\approxeq MON_2(p)$, the third multiplicative Zagreb connection index $M\hat{Z}C_3(\mathbb{F})$is,*
$M\hat{Z}C_3(\mathbb{F}) = 2.365399964090151e{+}26p^6 - 1.4192399784540906e{+}27p^5 + 3.5480999461352264e{+}27p^4 - 4.730799928180302e{+}27p^3 + 3.5480999461352264e{+}27p^2 - 1.4192399784540906e{+}27p + 2.365399964090151e{+}26.$

Proof. By using Defination 2.6.3:

$$M\hat{Z}C_3(\mathbb{F}) = \prod_{uv\in E(\mathbb{F})} [d_{\mathbb{F}}(u) \times \overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.6

$$\begin{aligned} M\hat{Z}C_3(\mathbb{F}) =&(3\times 4)(24)\times(3\times 5)(12)\times(3\times 5)(6p-6)\times(4\times 5)(12)\times(3\times 6)(12p-12)\times\\ &(4\times 6)(12p-12)\times(2\times 5)(6p-6)\times(3\times 6)(12p-12)\times(2\times 8)(12p-12)\times\\ &(3\times 9)(12p-12)\times(4\times 9)(12p-12)\end{aligned}$$

After solving it, we get our result:

$$\begin{aligned} =&2.365399964090151e+26p^6-1.4192399784540906e+27p^5+3.5480999461352264e+27p^4-\\ &4.730799928180302e+27p^3+3.5480999461352264e+27p^2-1.4192399784540906e+27p+\\ &2.365399964090151e+26.\end{aligned}$$

□

Theorem 3.4.10. *For the second metal organic network $\mathbb{F} \approxeq MON_2(p)$, the fourth multiplicative Zagreb connection index $M\hat{Z}C_4(\mathbb{F})$is,*
$M\hat{Z}C_4(\mathbb{F}) = 474141504149913600 0p^7-1896566016599654400 0p^6+2370707520749568000 0p^5-2370707520749568000 0p^3+1896566016599654400 0p^2-474141504149913600 0p.$

Proof. By using Defination 2.6.4:

$$M\hat{Z}C_4(\mathbb{F}) = \prod_{uv\in E(\mathbb{F})} [\overline{w}_{\mathbb{F}}(u) + \overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.5

$$\begin{aligned} M\hat{Z}C_4(\mathbb{F}) =&(3+4)(24)\times(3+5)(12)\times(4+5)(6p+6)\times(4+6)(12p)\times(5+5)(6p-6)\times\\ &(5+6)(12p-12)\times(5+8)(12p-12)\times(6+9)(12p-12)\times(8+9)(12p-12)\end{aligned}$$

After solving it, we get our result:

$$=47414150414991360000p^{7}-189656601659965440000p^{6}+237070752074956800000p^{5}-237070752074956800000p^{3}+189656601659965440000p^{2}-47414150414991360000p.$$

$\square$

Theorem 3.4.11. *For the second metal organic network $\mathbb{F} \approxeq MON_2(p)$, the modified first multiplicative Zagreb connection index $M\hat{Z}C_1^*(\mathbb{F})$ is,*
$M\hat{Z}C_1^*(\mathbb{F}) = 8.94227762957117e+27p^7 - 6.259594340699821e+28p^6 + 1.877878302209946e+29p^5 - 3.1297971703499102e+29p^4 + 3.1297971703499102e+29p^3 - 1.877878302209946e+29p^2 + 6.259594340699821e+28p - 8.94227762957117e+27.$

Proof. By using Defination 2.7.1:

$$M\hat{Z}C_1^*(\mathbb{F}) = \prod_{uv \in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(v) + d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(u)].$$

By using Table:3.6

$$\begin{aligned} M\hat{Z}C_1^*(\mathbb{F}) =& ((3)(4)+(2)(3))(24) \times ((3)(5)+(2)(3))(12) \times ((3)(5)+(2)(4))(6p-6) \times \\ & ((4)(5)+(2)(4))(12) \times ((3)(6)+(3)(4))(12p-12) \times ((4)(6)+(2)(4))(12) \times \\ & ((2)(5)+(3)(5))(6p-6) \times ((3)(6)+(3)(5))(12p-12) \times ((2)(8)+(4)(5))(12p-12) \times \\ & ((3)(9)+(4)(6))(12p-12) \times ((4)(9)+(4)(8))(12p-12) \end{aligned}$$

After solving it, we get our result:

$$=8.94227762957117e+27p^7 - 6.259594340699821e+28p^6 + 1.877878302209946e+29p^5 - 3.1297971703499102e+29p^4 + 3.1297971703499102e+29p^3 - 1.877878302209946e+29p^2 + 6.259594340699821e+28p - 8.94227762957117e+27.$$

$\square$

Theorem 3.4.12. *For the second metal organic network $\mathbb{F} \approxeq MON_2(p)$, the modified sec-*

ond multiplicative Zagreb connection index $M\hat{Z}C_2^*(\mathbb{F})$ *is,*
$M\hat{Z}C_2^*(\mathbb{F}) = 5.078630501577105e+27p^7 - 3.5550413511039732e+28p^6 + 1.0665124053311921e+29p^5 - 1.777520675551987e+29p^4 + 1.777520675551987e+29p^3 - 1.0665124053311921e+29p^2 + 3.5550413511039732e+28p - 5.078630501577105e+27.$

Proof. By using the Defination 2.7.2;

$$M\hat{Z}C_2^*(\mathbb{F}) = \prod_{uv\in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(u) + d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.6

$$\begin{aligned} M\hat{Z}C_2^*(\mathbb{F}) =& ((3)(3)+(2)(4))(24) \times ((3)(3)+(2)(5))(12) \times ((3)(4)+(2)(5))(6p-6)\times \\ & ((4)(4)+(2)(5))(12) \times ((3)(4)+(3)(6))(12p-12) \times ((4)(4)+(2)(6))(12)\times \\ & ((2)(5)+(3)(5))(6p-6) \times ((3)(5)+(3)(6))(12p-12) \times ((2)(5)+(4)(8))(12p-12)\times \\ & ((3)(6)+(4)(9))(12p-12) \times ((4)(8)+(4)(9))(12p-12) \end{aligned}$$

After solving it, we get our result:

$$\begin{aligned} =& 5.078630501577105e+27p^7 - 3.5550413511039732e+28p^6 + 1.0665124053311921e+29p^5 - \\ & 1.777520675551987e+29p^4 + 1.777520675551987e+29p^3 - 1.0665124053311921e+29p^2 + \\ & 3.5550413511039732e+28p - 5.078630501577105e+27. \end{aligned}$$

□

Theorem 3.4.13. *For the second metal organic network* $\mathbb{F} \approxeq MON_2(p)$*, the modified third multiplicative Zagreb connection index* $M\hat{Z}C_3^*(\mathbb{F})$ *is,*
$M\hat{Z}C_3^*(\mathbb{F}) = 1.8545024515607018e+37p^7 - 1.2981517160924912e+38p^6 + 3.894455148277474e+38p^5 - 6.490758580462456e+38p^4 + 6.490758580462456e+38p^3 - 3.894455148277474e+38p^2 + 1.2981517160924912e+38p - 1.8545024515607018e+37.$

Proof. By using Defination 2.7.2:

$$M\hat{Z}C_3^*(\mathbb{F}) = \prod_{uv \in E(\mathbb{F})} [d_{\mathbb{F}}(u)\overline{w}_{\mathbb{F}}(u) \times d_{\mathbb{F}}(v)\overline{w}_{\mathbb{F}}(v)].$$

By using Table:3.6

$$\begin{aligned} M\hat{Z}C_3^*(\mathbb{F}) =& ((3)(3) \times (2)(4))(24) \times ((3)(3) \times (2)(5))(12) \times ((3)(4) \times (2)(5))(6p-6) \times \\ & ((4)(4) \times (2)(5))(12) \times ((3)(4) \times (3)(6))(12p-12) \times ((4)(4) \times (2)(6))(12) \times \\ & ((2)(5) \times (3)(5))(6p-6) \times ((3)(5) \times (3)(6))(12p-12) \times ((2)(5) \times (4)(8))(12p-12) \times \\ & ((3)(6) \times (4)(9))(12p-12) \times ((4)(8) + (4)(9))(12p-12) \end{aligned}$$

After solving it, we get our result:

$$\begin{aligned} =& 1.8545024515607018e+37p^7 - 1.2981517160924912e+38p^6 + 3.894455148277474e+38p^5 - \\ & 6.490758580462456e+38p^4 + 6.490758580462456e+38p^3 - 3.894455148277474e+38p^2 + \\ & 1.2981517160924912e+38p - 1.8545024515607018e+37. \end{aligned}$$

$\square$

Chapter 4

Conclusion

In this thesis we studied history, definition of that terms which is useful to understand the structures such as (Graph, Subgraph, Size and Order of Graph, Degree of Vertex, Isolated Vertex, Pendent Vertex, Odd Vertex, Even Vertex, Adjacent Vertices, Neighborhood of Vertices, Adjacent Edges, Pendent Edges, simple Graph, Multiple Graph, Finite Graph, Infinite Graph, Cyclic graph, Regular Graph, Planar and Non-Planar Graph, Walk, Path, Operations on Graph). Then we discussed the structures and its formation. After that, we studied some distance based topological indices and in this thesis we computed the Zagreb connection based indices for metal-organic networks.

Chapter 5

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