Merrifield-Simmons Index of Molecular Graphs

By

Noor-un-Nisa

CIIT/FA16-RMT-014/LHR

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Name	Registration Number
Noor-un-Nisa	CIIT/FA16-RMT-014/LHR

Supervisor

Dr. Hani Shaker

Associate Professor, Department of Mathematics

COMSATS University Islamabad, Lahore Campus

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Final Approval

This report titled

Merrifield-Simmons Index of Molecular Graphs

By

Noor-un-Nisa

CIIT/FA16-RMT-014/LHR

Has been approved

For the COMSATS University Islamabad,Lahore Campus

ExternalExaminer:______________________________

Dr. Kashif Shafiq

Supervisor: _____________________________

Dr. Hani Shaker

Department of Mathematics /CUI, Lahore Campus

HoD:___________________________________

Department of Mathematics, Lahore Campus

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CIIT/FA16-RMT-014/LHR

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It is certified that **<u>Noor-un-Nisa (CIIT/FA16-RMT-014/LHR)</u>** has carried out all the work related to this thesis under my supervision at the Department of Mathematics, COMSATS University Islamabad, Lahore Campus, and the work fulfills the requirement for award of MS degree.

Date:__________________

Supervisor:

____

Dr. Hani Shaker
Associate
Professor

Head of Department:

____

Dr. Sarfraz Ahmed
Associate Professor
Department of Mathematics

DEDICATION

To

My dearest husband

ACKNOWLEDGEMENTS

First and Foremost I am thankful to Allah Almighty the most Gracious and the most merciful, Who gave me the stability and strength to complete this thesis. Without His blessing I wouldn't be able to do anything. My very modest praise is due to the beloved Holy Prophet Muhammad S.A.W whose love is light to me.
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Noor-un-Nisa
CIIT/FA16-RMT-014/LHR

ABSTRACT

Merrifield-Simmons Index of Molecular Graphs

The main objective of this thesis is to compute Merrifield- Simmons index of molecular graphs. The molecular graph that is taken for this purpose is V- phenlynic graph. The nanostructures under consideration are nanosheet $G = VPHY[p,q]$ and $H = VPHZ[p,q]$ nanotube. We compute the results for V- phenlynic nanosheet and nano tube. To compute Merrifield- Simmons index, first we find all independent sets of said graphs. We use the technique of transfer matrix to solve this problem. We develop some algorithms to compute Merrifield- Simmons index of said graphs. We construct a matlab program for the final results.

Table of Contents

List of Figures

Chapter 1

Introduction

Graph theory is known as the study of graphs, which is well-known field of Discrete Mathematics. The applications and developments of graph theory are not limited to the field of mathematics, but also to the different fields of Biology, Physics, Chemistry, Computer Science, Technology, and Social Sciences. They provide us efficient tools which may be used to solve different types of problems in various mathematical fields. Consider the fig. 1.1 which describe a portion of road map.

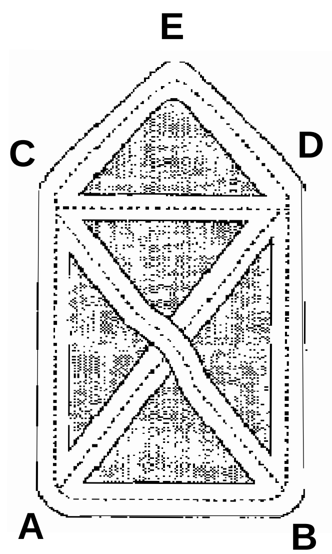

Figure 1.1: *Road Map*

while studying chapter 2, we would discuss some important definitions related to graphs. Different types of graphs that include complete graph, regular graph, bipartite graph etc will be a part of this chapter. Mathematical operations applied to two different graphs will be discussed. A very important term related to research work of this thesis i.e. independent sets will be studied in this chapter.

In chapter 3, we will discuss about Mathematical Chemistry. Mathematics also has experimental roots like as Chemistry. The combination of Mathematics and Chemistry introduced formally in last century which is known as Mathematical Chemistry. The role of Mathematics in chemistry is of great importance as it provides a way to understand the chemical structures.We can say that the chemical graph theory may be the branch of Mathematical Chemistry. This branch of Mathematics is developing fast. Graph theory is helpful to get different chemical structures mathematically to study their physical characteristics. In 2008, A book on "Some New Trends in Chemical Graph Theory" is published [8]. We are working on molecular graphs. Molecular graph consists of atoms and bond. These include non hydrogen atoms and covalent bonds.

In chapter 4, we will discuss topological descriptors. Molecular Descriptors are used to investigate a chemical structure. These can be in different forms like numbers or matrices that describe the properties of molecules. One of the interesting topological descriptor is topological indices. There are many types of topological indices that are based on different classes. The topological index in which we are doing this thesis is Merrifield- Simmons index.

Chapter 5, is the last chapter that is about our main results. The chemical structure which is selected for this research is V-Phenlynic. Our main aim is to compute Merrifield- Simmons index for V- Phenlynic nanosheet and nanotube. The results are computed with the help of algorithm which is developed by me. At the end there will be concluding remarks.

Chapter 2

Graph Theory and Its Preliminaries

In this chapter, we will study about graphs and the terms related to graph and graph theory. These terms will help us to understand this subject in better way. Moreover these terminologies are also helpful and played an important role in our research which is conducted in this thesis. There are many types of graphs depend on their structure. We can also apply some operations to two different graphs. Different types of graphs and operations on graphs will also be studied in this chapter. We will also give some examples which explain our definitions and terminologies.

2.1 Graph

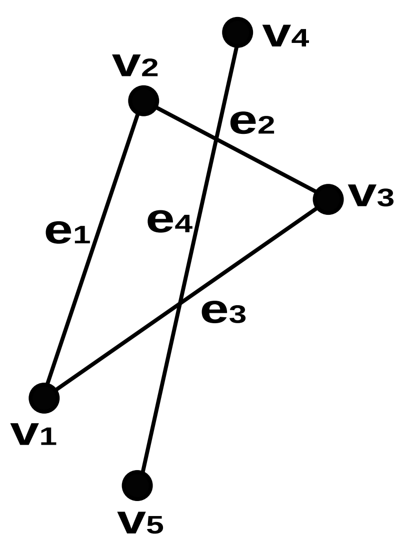

Figure 2.1: *Graph G*

Definition 2.1. Graph

As a mathematical object a graph G is considered as a pair of sets, one is set of nodes, known vertices $V(G)$ and a set of links between the nodes called edges $E(G)$. Usually, G is written like $G = (V(G), E(G))$, but in short we write it as G.

Definition 2.2. Order of the graph

The cardinality $|V|$ is represented by m, where m is called order of the graph G.

Definition 2.3. Size of the graph

The cardinality $|E|$ is denoted by n, where n is size of graph G.

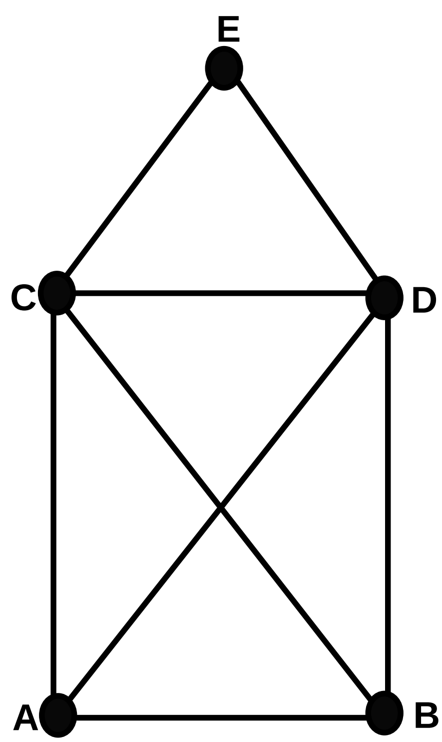

Figure 2.2: *Graph* G_1

Example 2.1.1. *Consider a graph G=G(V,E) as shown in fig 2.1:*

In this graph V=V(G)=$\{v_1,v_2,v_3,v_4,v_5\}$ *is the vertex set and edge set is E=E(G)=*$\{e_1, e_2, e_3, e_4\}$.

Size of graph G is 5. i.e m=5. Order of graph G is 4 i.e n=4.

Here is the graph representation of road map as given in previous chapter see, fig. 2.2. *A, B, C, D, E* are the vertices and the edges between vertices are represented by lines. It is also noted that the intersection of edges AD and BC is not a vertex as cross-roads do not exist in the diagram.

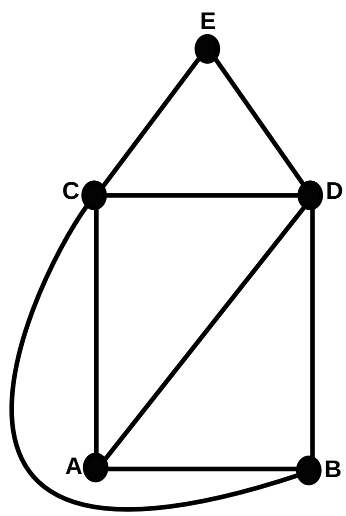

Figure 2.3: *Graph* G_2

Moreover, if we draw a line BC outside the rectangle $ABCD$ in fig. 2.3, then the resulting graph tells us the same situation as in fig. 2.2 . This graph also represents the direct road from B to C but the length of road is changed now. A graph tells us the features of structure by how we join the points by lines.If the vertices joined by a line known as edge in graph I are same as corresponding vertices joined by a line in graph say F then these two graphs are said to be the same graphs. The graphs in fig. 2.2 and fig. 2.3 are the same graphs.

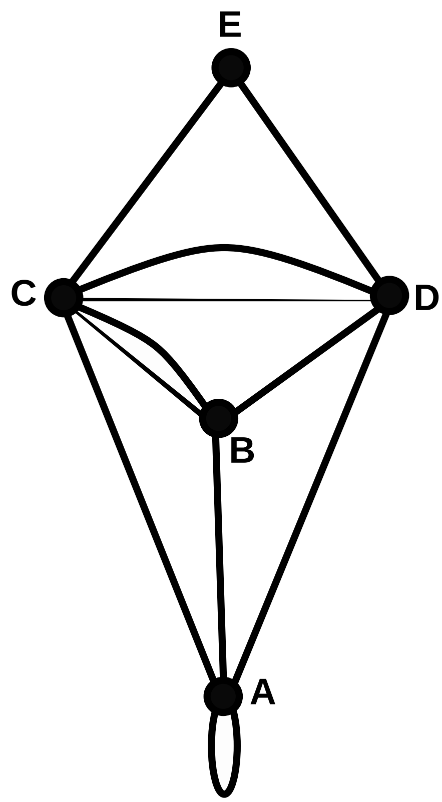

Figure 2.4: *Graph G_3*

In the fig 2.3, here is a graph having at most single edge between every pair of vertices. Now, suppose that the flow of traffic is high on the roads representing edges CD and BC. To solve this problem by making extra roads among them. This terminology is known as **multiple** edges. Suppose that we need a small park at the point A. So, this situation is handled by having an edge from vertex A to itself. This is called **loop** as shown in fig 2.4. Also,Any Two vertices may be known as **adjacent** if there is a line between them.

Definition 2.4. Degree of a vertex

Total number of edges with a same vertex called degree of that same vertex. if v is a vertex then its degree is represented by *d(v)* or *deg(v)*.

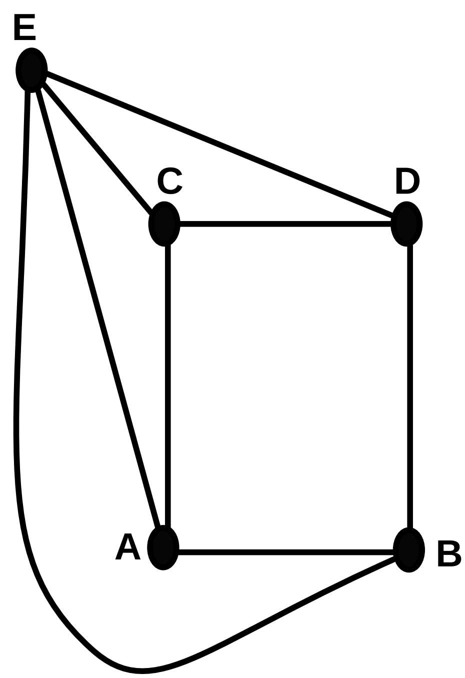

Figure 2.5: *Graph* G_4

Example 2.1.2. *Consider a graph G=(V(G),E(G) as shown in fig 2.5. In this graph:*

d(A)=3

d(B)=3

d(C)=3

d(D)=3

d(E)=4

2.2 Types of Graph

There are many types of graphs that are based on their structure. Some of them are discussed below.

Definition 2.5. Null graph

A graph that does not have any edge is called null graph.

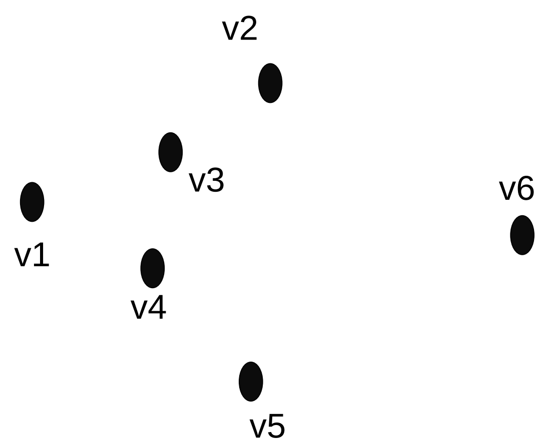

Figure 2.6: *Null graph*

Example 2.2.1. *Choose a graph shown in fig. 2.6. There is no edge between any two nodes or vertices in graph. It is known as null graph.*

Definition 2.6. Simple graph

If a graph$E$ having no loops and multiple edges then graph$E$ is said to be a simple graph.

Example 2.2.2. *Choose the graphs shown in fig. 2.7. These are some example of simple graphs. Note that there are no loops and multiple edges in these graphs.*

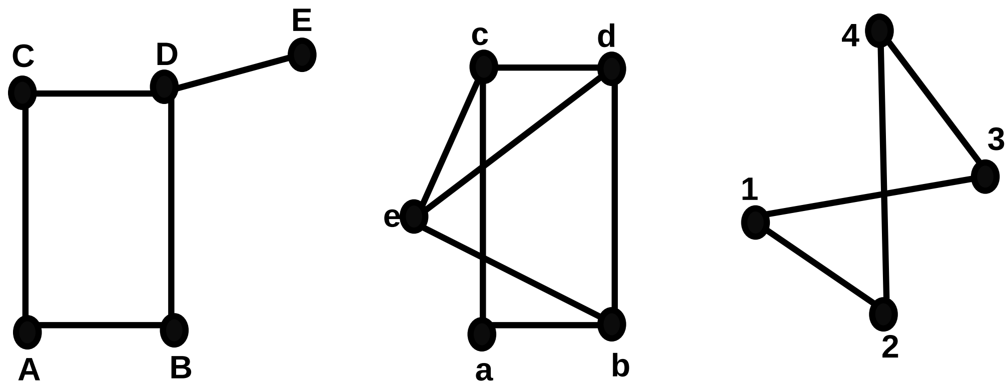

Figure 2.7: *Simple graphs*

Definition 2.7. Non simple graph

If there a graph$E$ having loops and multiple edges then graph$E$ represent to a non simple graph.

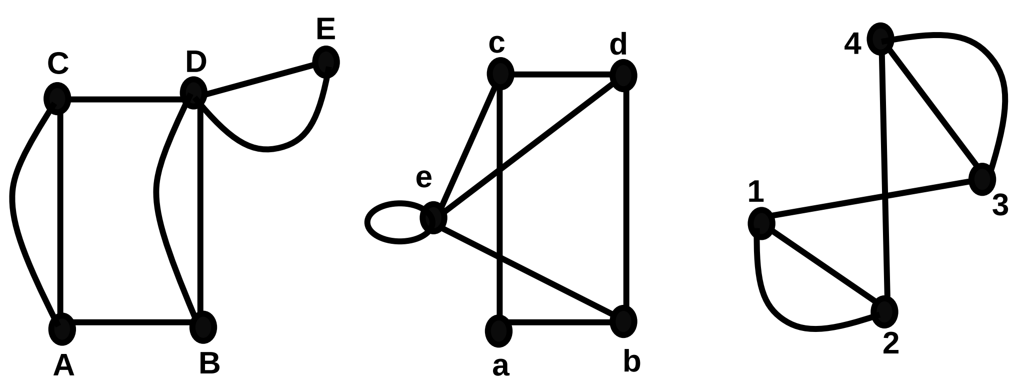

Figure 2.8: *Non Simple graphs*

Example 2.2.3. *Choose the graphs shown in fig. 2.8. These are some example of non simple graphs. Note that there are loops and multiple edges in these graphs.*

Definition 2.8. Directed graph

If some direction is given to the edges then it is called directed graph. This type of graph is more explanatory than others. The concept of in-degree and out-degree of a vertex is also related to the directed graphs.

Definition 2.9. In- degree of a vertex

The number of incident lines coming upward to any vertex$e$ is called in- degree of a vertex$e$.

Definition 2.10. Out- degree of a vertex

The number of incident lines coming downward to any vertex$e$ is called out- degree of a vertex$e$.

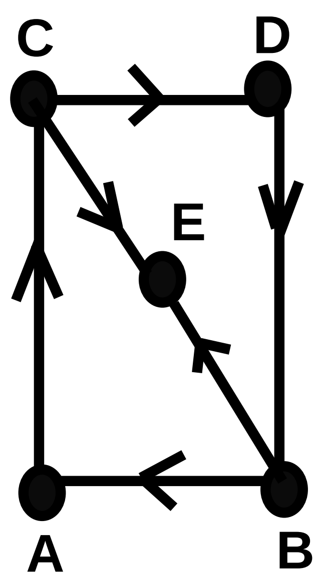

Figure 2.9: Directed graph

Example 2.2.4. *Choose the graphs shown in fig. 2.9. The direction is given to every vertex in this graph. In- degree of a vertex C is 1, out- degree of a vertex C is 2 and total degree of vertex C is 3.*

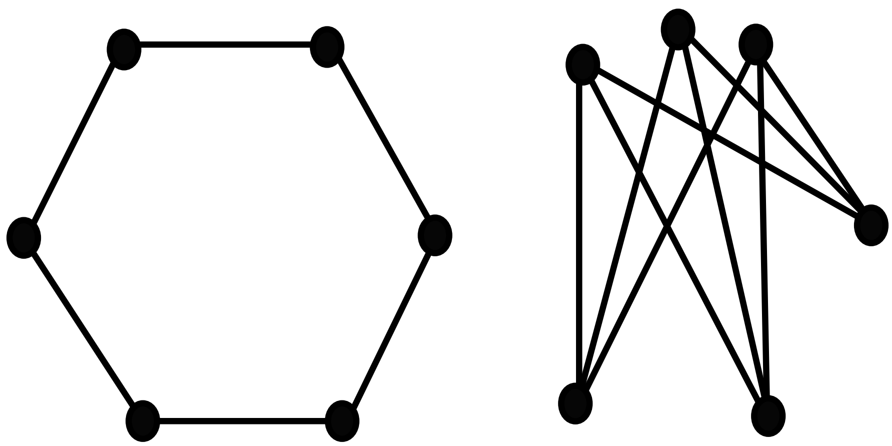

Figure 2.10: 2-regular and 3-regular

Definition 2.11. Regular graph

All vertices of a graph having the same degree is known as a regular graph. If every vertex of a graph has degree s, then it is known *s-regular*.

Example 2.2.5. *The 2-regular and 3-regular graphs are shown in fig 2.10.*

Definition 2.12. Path graph

If we remove an edge from cyclic graph C_n then the resulting graph is known as path graph on n number of vertices. It is denoted by P_n.

Example 2.2.6. *The graphs representing P_3, and P_5 are shown in fig 2.11.*

Figure 2.11: P_3 and P_5

Definition 2.13. Cycle graph

A *2-regular* connected graph is said to be a cycle graph. Cycle graphs with n number of vertices are denoted by C_n.

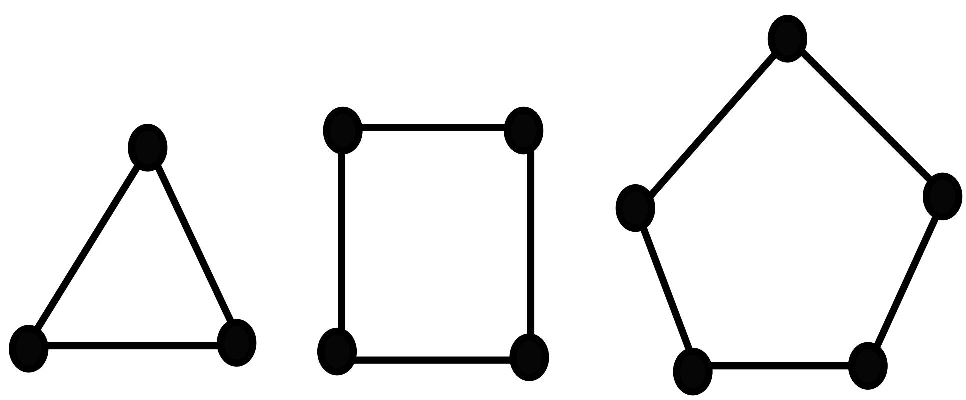

Figure 2.12: C_3, C_4 *and* C_5

Example 2.2.7. *The graphs representing* C_3, C_4 *and* C_5 *are shown shown in fig 2.12.*

Definition 2.14. Connected graph

Any graph$G$ is known as a connected graph if it has a path between any two vertices.

Definition 2.15. Disconnected graph

Any graph$G$ is known as a disconnected graph if it has no path between any two vertices.

Definition 2.16. Complete graph

A graph is said to be complete graph if every vertex is linked with any other vertex by an edge. Complete graphs on n-number of vertices are denoted by K_n.

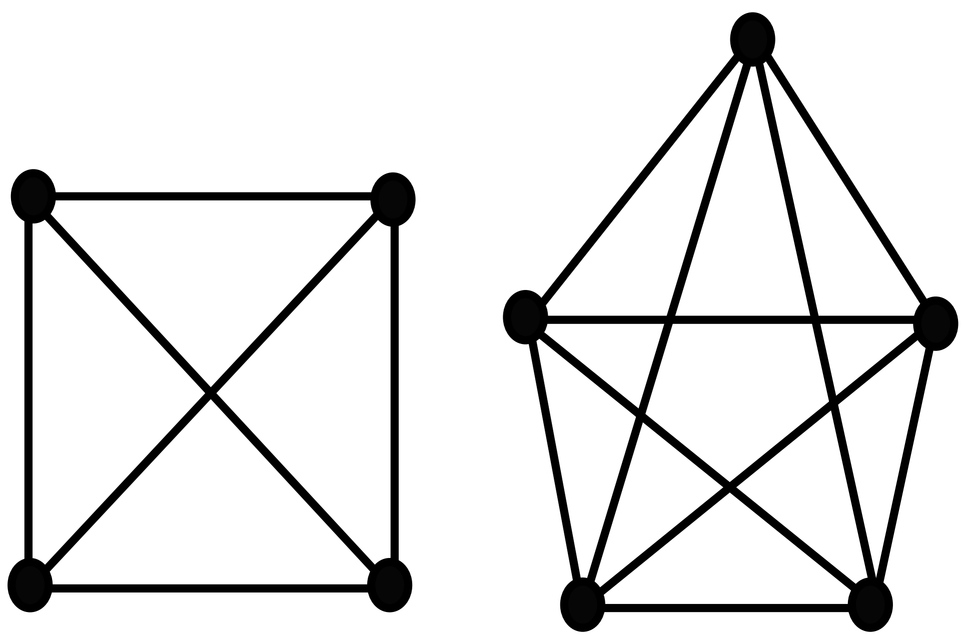

Figure 2.13: K_4 *and* K_5

Example 2.2.8. *The graphs representing* K_4 *and* K_5 *are shown in fig 2.13.*

Definition 2.17. Wheel

The graph came from C_{n-1} by joining every vertex to a new vertex v. The resulting graph of n number of vertices is called wheel and is denoted by W_n.

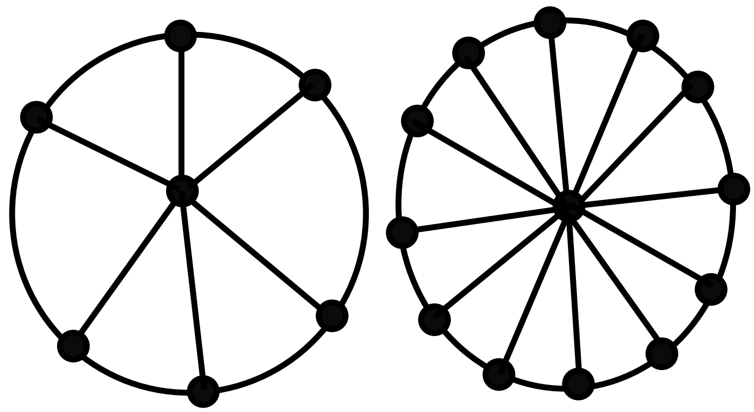

Figure 2.14: W_4 *and* W_5

Example 2.2.9. *The graphs representing* W_4*, and* W_5 *are shown in fig 2.14.*

Definition 2.18. Bipartite graphs

Consider M=$\{a,b,c\}$ and N =$\{e,f\}$ are two disjoint vertex sets. If each vertex of set A is linked with vertex of set B. Then the graph is said a bipartite graph. Note that no vertex of set A is linked with any other vertex of set A. Similarly no vertex of set B is linked with any other vertex of set B. We can color vertex set A to white and vertex set B to black.

Example 2.2.10. *The 2-regular, and 3-regular graphs are shown in fig 2.15.*

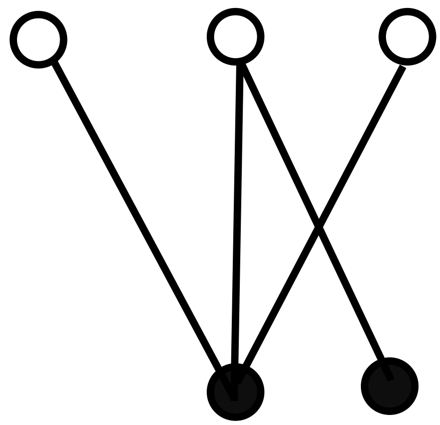

Figure 2.15: *Bipartite graph*

Definition 2.19. Complete Bipartite graphs

A complete bipartite graph having every vertex in M is joined to each vertex in N by only single edge is known as bipartite graph. If we color x to white and y to black vertices, then bipartite graph is represented by $K_{x,y}$.

Example 2.2.11. *The $K_{1,3}$, and $K_{2,3}$ graphs are shown in fig 2.16.*

Definition 2.20. Cyclic graph

A graph that contain minimum one cycle is said to be a cyclic graph.

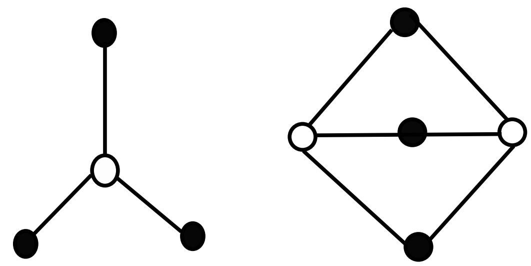

Figure 2.16: $K_{1,3}$ *and* $K_{2,3}$

Definition 2.21. Acyclic graph

A graph without any cycle is said to be acyclic graph.

Definition 2.22. Tree graph

A connected graph with no cycle is said to be tree graph or tree.

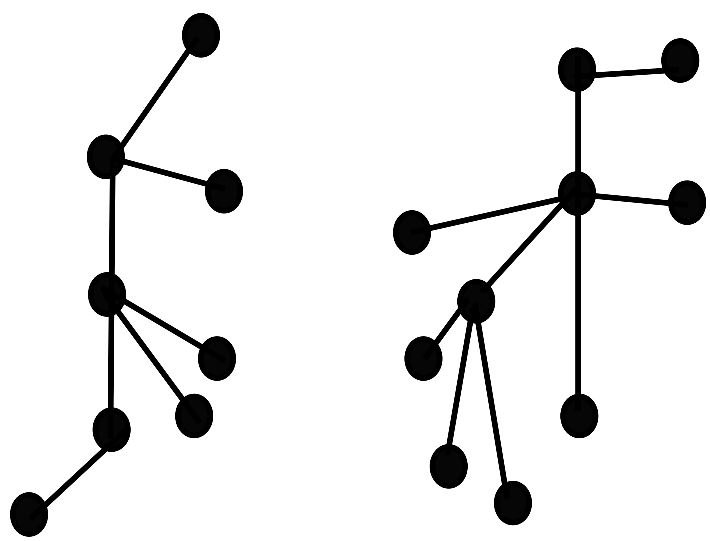

Figure 2.17: *Tree graph*

Example 2.2.12. *The tree graphs shown in fig 2.17.*

Definition 2.23. Isomorphic graphs

Two graphs G and $G^{'}$ are said to be isomorphic if there exists a function $\varphi : V(G) \to V(G^{'})$ such that any two vertices u and $u^{'}$ of G are adjacent in G iff f(u) and $f(u^{'})$ are adjacent in $G^{'}$. If two graphs G and $G^{'}$ are isomorphic then these two graphs are called isomorphic graphs and are denoted by $G \cong G^{'}$.

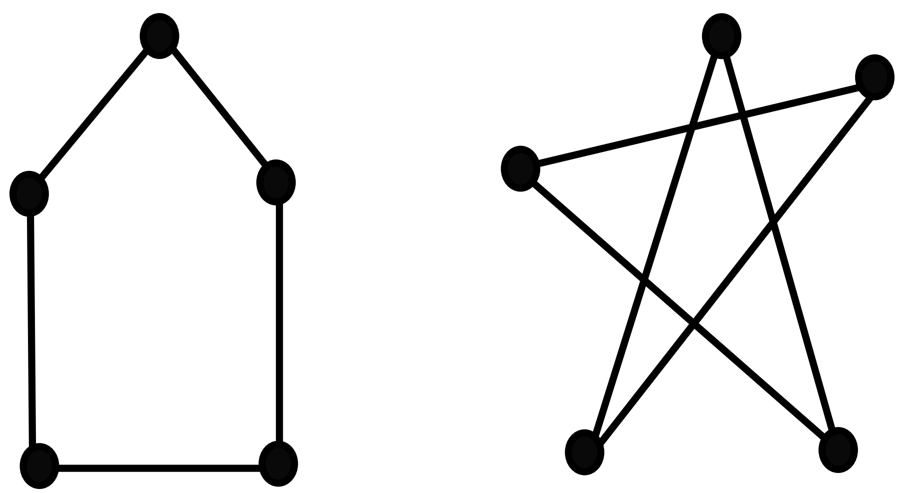

Figure 2.18: G and $G^{'}$

Example 2.2.13. *Consider the graphs in fig 2.18. These two graphs are isomorphic.*

2.3 Operations on Graphs

As, we discussed about graph as a Mathematical objects, likely to other mathematical objects. One may think about some operations that can be apply to two graphs to construct new graph. In this section, we will discuss some operations of graphs.

Some of the operations are:

Definition 2.24. Union of graphs

Let G and $G^{'}$ be two graphs. The union of G and $G^{'}$ is denoted by $G = G \cup G^{'}$. It consists of the vertex set $V(G) \bigcup V(G^{'})$ and the edge set $E(G) \cup E(G^{'})$.

Example 2.3.1. *Choose the graphs in fig 2.19. This shows the union of two graphs $G \cup G^{'}$.*

Definition 2.25. Intersection of graphs

Let E and $E^{'}$ be two graphs. The intersection of E and $E^{'}$ is represented by $E = E \cap E^{'}$. It carries the vertex set $V(E) \cap V(E^{'})$ and the edge set $E(E) \cap E(E^{'})$.

Example 2.3.2. *Choose the graphs in fig 2.20. This shows the intersection of two graphs $G \bigcap G^{'}$.*

Definition 2.26. Complement of graphs

The complement of a graph is represented by $\bar{G}$. It is a graph with vertex set V(G)=V($\bar{G}$) such that two vertices of $\bar{G}$ iff they are not adjacent in G.

Example 2.3.3. *Choose the graphs in fig 2.21. This shows the complement $\bar{G}$ of graph G.*

2.4 Independent set

Definition 2.27. Independent set

Let G be a graph then an independent set $I(G)$ is defined as subset of vertex set of graph G such that $I(G)$ does not contain two adjacent nodes. see fig 2.22

2.4.1 History

In 1931, Konig's Thm published the result, the number of vertices are always equal to the size of the maximum independent set plus the size of the maximum matching. In 1995, In graphs having at most one cycle, maximal independent sets is published [11] In 1960, Miller and Muller published the result, bound on maximum number of maximal independent sets in a graph.

In 1995, A survey [7] on counting maximal independent sets is published. After that in 2000, they [6] also published results of independent sets. In 1998, [5] The number of independent sets in a grid graph computed.

In 2005, [15] The number of independent sets in unicyclic graphs computed. The number of independent sets in trees also computed in this year [10].

P.D. Vestergaard and Pederson found some results regarding independent sets [16].

Example 2.4.1. *Consider the graph in fig 2.23:*

This is a simple graph. We can see that vertices a, b, c and d are independent vertices. The vertices a and b, also vertices c and are independent as there is no edge between them. There is no independent set between three vertices.

Example 2.4.2. *Choose the graph shown in fig 2.24:*

There are many independent sets. There is no edge between vertices a and b, a and c, and a and f, so these are also elements of an independent set. Vertices a, d, b and f also make independent set.

Definition 2.28. n-independent sets

An independent set on m number of vertices is said n-independent set.

(1) independent set is independent set of single vertex.

(2) independent set is independent set of two vertices.

(3) independent set is independent set of three vertices. So

(m) independent set is independent set of n vertices.

Example 2.4.3. *Consider a graph in fig 2.25: 1- independent set:* $\{a\}$, $\{b\}$, $\{c\}$, $\{d\}$, $\{e\}$, $\{f\}$

2- independent set: $\{b,c\}$, $\{c,d\}$, $\{d,e\}$, $\{e,f\}$, $\{f,b\}$

3- independent set:$\{b,c,d\}$, $\{b,d,e\}$, $\{b,e,f\}$, $\{b,c,e\}$, $\{b,c,f\}$, $\{b,d,f\}$, $\{b,e,f\}$, $\{c,d,e\}$, $\{c,d,f\}$,$\{c,e,f\}$, $\{d,e,f\}$

4- independent set: $\{b,c,d,e\}$, $\{b,c,d,f\}$, $\{b,d,e,f\}$, $\{c,d,e,f\}$

5- independent set: $\{b,c,d,e,f\}$

Definition 2.29. Independent Number

The cardinality of maximal independent set in a graph G is called independent number. For example, in previous graph independent number is 5.

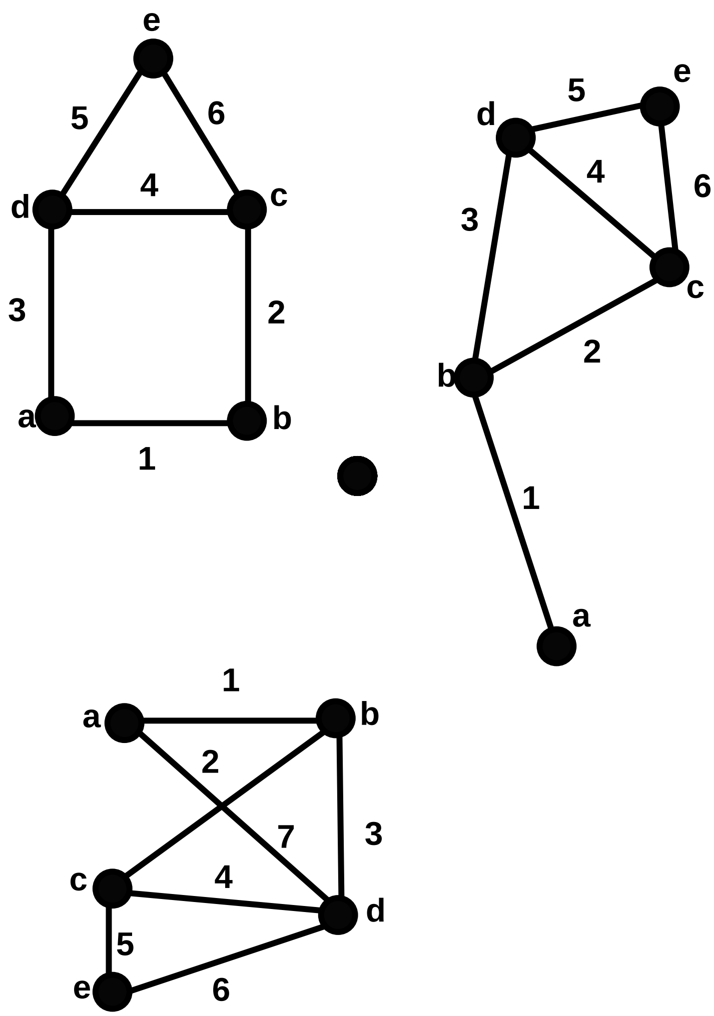

Figure 2.19: $G = G \cup G'$

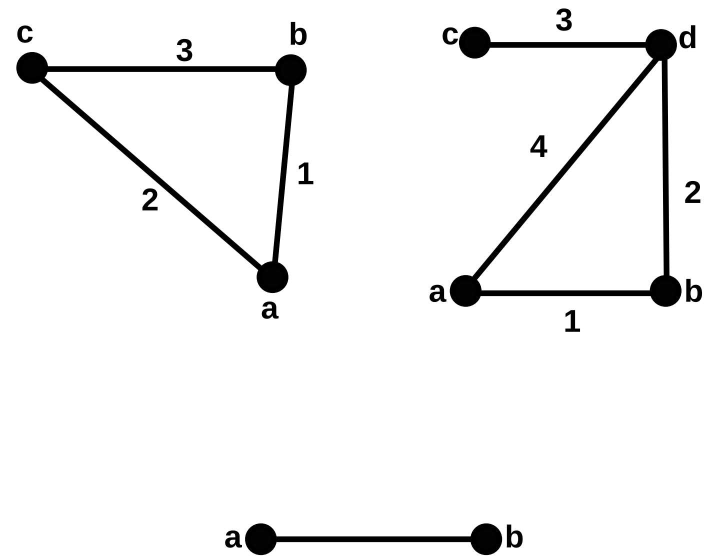

Figure 2.20: $E = E \cap E'$

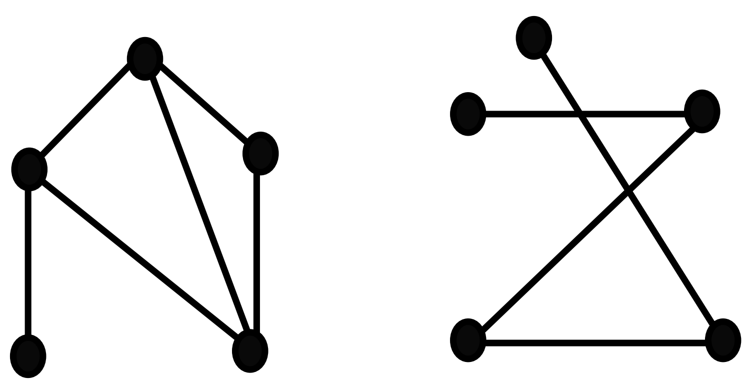

Figure 2.21: G *and* $\bar{G}$

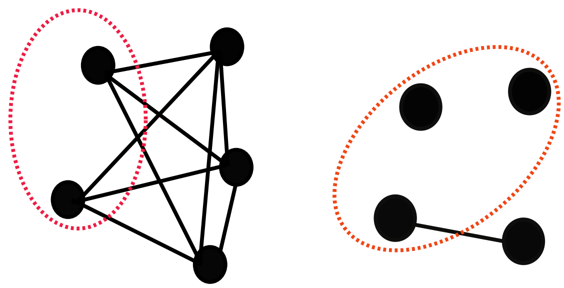

Figure 2.22: *Graph G'*

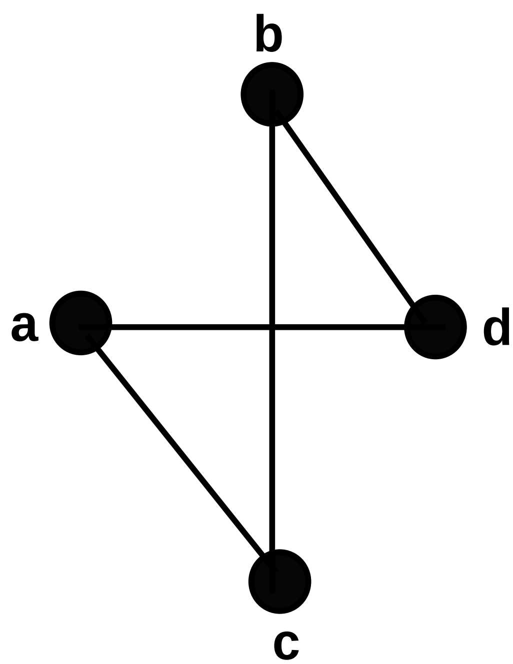

Figure 2.23: Graph G''

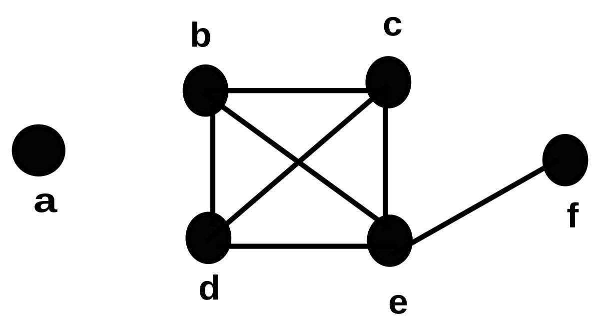

Figure 2.24: *Graph* G'''

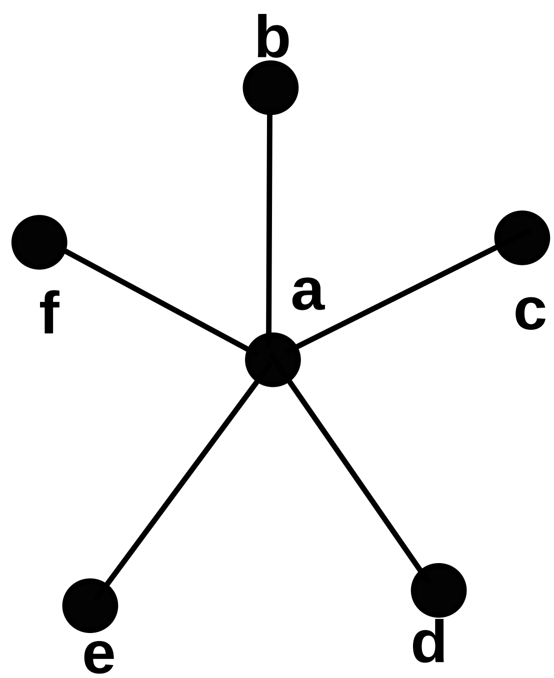

Figure 2.25: *Graph* G^*

Chapter 3

Chemical graph theory

3.1 Mathematical Chemistry

Mathematics is the tool that is used in every field of life. It is the mother of all sciences because it is a gadget to solve problems. Without it, we cannot understand either physics, chemistry, biology or any other sciences. Mathematics is the most efficient term that formulate the theories of natural sciences. Chemistry is also exists every where. Bodies are manufactured by molecules. Without Chemistry, there is no possibility of any human activity. Mathematics also has experimental roots like as Chemistry. The combination of Mathematics and Chemistry introduced formally in last century which is known as Mathematical Chemistry. The role of Mathematics in chemistry is of great importance as it provides a way to understand the chemical structures. It is the field of research which used applications of mathematics into chemistry. In 1894, Georg Helm first published treatise with title "The Principles of Mathematical Chemistry: The Energetics of Chemical Phenomena". For the time being, Mathematical problems may be solved by Chemical procedures. Till now a lot of work has been done on Mathematical chemistry. In 2001, Nenad and Gutman briefly described the roots of Mathematics and Chemistry [18]. Balaban wrote about reflection on Mathematical Chemistry in 2005[3]. Mathematic has many diverse areas such as group theory, differential equations,functional analysis, group theory, topology, combinatorics,Hilbert spaces and many more. Some of these areas are very fruitful for chemistry. The areas of Mathematical chemistry include Electrochemistry, Mathematical crystallography, Ab initio quantum chemistry, Chemical reaction-network analysis, Chemo-metrics and QSAR, Molecular biology, Chemical graph theory and many more [9]. The area of our interest is Chemical Graph Theory.

3.2 Chemical Graph Theory

A field of Mathematics that merge graph theory and chemistry is known as chemical graph theory. This branch of Mathematics is developing fast. Graph theory is used to model different chemical structures mathematically to study their physical characteristics. Some of the problems in Graph theory are very simple to formulate and understand but on the same side many problems are difficult to understand and also it is very difficult to find their solutions. If we raise a question about the combination of chemistry and graph theory that how can we describe Graph theory elements in term of Chemistry then the answer would be given by following example i.e. Theorem of Graph Theory:

Any graph contains an even number of vertices of odd degree.

The conversion of this theorem in chemical language is:

Every molecule contains an even number of atoms of odd valence.

3.2.1 History and development of Chemical Graph theory

Nenad Trinajstic is one of the pioneer of Chemical Graph Teory. His contribution in the development of Chemical Graph Theory has to be appriciated since early 1970s to today. There other pioneer of Chemical Graph Theory are Haruo Hosoya, Alexendru T. Balaban, Ivan Gutman. D.J. Klein and Milan Randic has also participate in this field. In 1976, Balaban came up with the first book on application of Graph theory to Chemistry [4]. The scope of Chemical graph theory is rapidly increasing. In 2008, A book on "Some New Trends in Chemical Graph Theory" is published [8]. Valence and cubic graph, Valene derivatives, Benzenoid polycyclic hydrocarbons, diamondoid hydrocarbons, cospectral graphs and isoprenoid structures are some chemical applications of graph theory discussed in [2]. King and R. Bruce was also interested in applications [12].

3.3 Molecular Graphs

In this section, we will study about chemical graphs and their characteristics. We will some examples of molecular graphs that occur in mathematical investigation.

Definition 3.1.

A graph representing the structural formula for chemical compound in terms of graph theory. The non-hydrogen atoms are defined by vertices and the edges define covalent bonds among these atoms.

Definition 3.2.

The elements of molecular graph are:

- Atoms
- Bonds

Atoms are represented as the vertices and bonds are represented as the edges among these atoms.

In 1874, Arthur Cayley was the first who discussed molecular graph in his results. Molecular graphs are convenient way to understand a chemical structure.

Example 3.3.1. *Consider the Chemical structure as shown in fig 2.1:*

The skeleton graph represents only those atoms which can be regarded as forming the framework of the molecule. Other atoms, which are usually hydrogens, are disregarded. The skeleton graph is almost universally used in applications of graph theory to saturated and fully conjugated hydrocarbons, since then the neglect of the hydrogen atoms cannot cause any ambiguity.

The first of them represents cyciohexane, the second methylcyciopentane, the third 1,1-dimethylcyciobutane, etc. The skeleton graphs of fully conjugated molecules, not necessarily hydrocarbons, are called HDcKEL graphs because of their role in HDcKEL molecular orbital theory.They correspond, in fact, to the network over which the n-electrons in such molecules are delocalized.

Here are some examples: Some special types of graphs have been used in the topo-

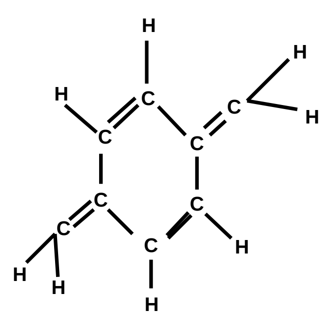

Figure 3.1: *Molecular graph 1*

logical investigations of benzenoid hydrocarbons. The inner dual is obtained by associating a vertex to each hexagon and connecting vertices corresponding to adjacent hexagons. The inner dual of benzo

a

pyrene is given as follows:

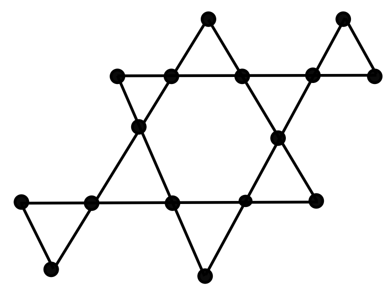

Figure 3.2: *Molecular graph 2*

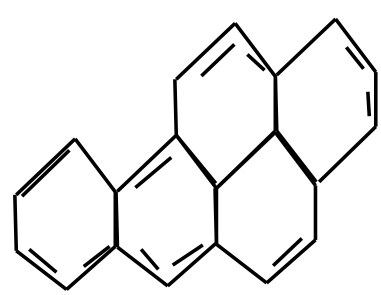

Figure 3.3: *Molecular graph 3*

Chapter 4

Topological Descriptors

4.1 Introduction

Topological descriptors played an important role in chemical graph theory. Molecular Descriptors are used to investigate a chemical structure. These can be in different forms like numbers or matrices that describe the properties of molecules. Molecular Descriptors are based on Quantum Mechanics, which provide accuracy of our results but on the same side there computation is time consuming. Moreover, the simple molecular descriptors are based on easy counts of characteristics such as hydrogen bond donors, hydrogen bond acceptors, molecular weight, rotatable bonds and molecular weight. In this chapter, we will study about topological descriptors, its different types those are depend on the dimensions. Next, we will have one of the topological descriptor i.e. topological indices. There are different classes of topological indices and at the end we will briefly describe Merrifield-Simmons index which is the main topological index of our thesis.

4.2 Topological Descriptors

Definition 4.1.

The molecular descriptor is the final result of a logic and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment.

Topological descriptors are divided into different types depending upon the dimensionality of molecular structure. These types are as follows:

- 1D: Based on the types of atom which make molecule

- 2D: Based on the bonding of molecule
- 3D: Based on the spacial arrangement of molecule

There are many types of topological indices. These types give us results about molecular structure. Different types of topological descriptors include matrices, polynomials, sequences and indices. One of the famous and powerful type of topological descriptor is Topological indices.

4.3 Topological Indices

When molecular property associates with the topological descriptors then we have a topological index. It is also called molecular index. The topological index convert a chemical structure into a single number. It is very useful in the field of QSPR/QSAR. More than hundred topological indices introduced that study different types of molecular structures.

4.3.1 Classification

There are two main classes of Topological indices. These include

- Distance-based Topological Indices
- Degree-based Topological Indices

The degree-based Topological indices include

- Zagreb Indices
- Narumi-Katayama and Multiplicative Zagreb Indices

- Atom-bond Connectivity Index
- Augmented Zagreb Index
- Geometric-arithmetic Index
- Harmonic Index
- Sum-connectivity Index

The distance-based Topological indices include

- Wiener index
- Harary index
- Total eccentricity index
- Hosoya index

Other than these two classes there is another class of indices that based on the number of certain components of given graph. One of these types of index is Merrifield-Simmons index.

4.4 Merrifield-Simmons index

Let $G = G(V, E)$ be a graph then an independent set $I(G)$ is defined as subset of vertex set of graph G such that $I(G)$ does not contain two adjacent nodes. The total number of independent sets of graph G is known as Merrifield-Simmons index and is denoted by σ.

4.4.1 History and development

In 1960 Miller and Muller written about calculating maximal independent sets in a graph. In their first paper in 1980 about the structure of molecular topological space Merrifield and Simmons used the symbol σ for this quantity. After that Prodinger and Tichy gave motivation to the study of the number of independent sets $I(G)$ in chemical graph theory in 1982.The Merrifield-Simmons index is proposed by R. E. Merrifield and H. E. Simmons in 1989. After that it was accepted by the whole mathematico-chemical community. The index σ was not named in the two early papers of Gutman in 1992.Gutman first named this index the Merrifield-Simmons index in 1993.Many chemical applications can be found in 1989 by Merrifield and Simmons [13]. For example, in [14] it was shown that $I(G)$ is associated with boiling points. An analysis on calculating maximal independent sets is provided by Chou and Chang in 1995. In recent years a great work has been done on this index. The Merrifield-Simmons index of simple and cyclic graphs are computed by M. B. Ahmadi and H. Dastkhezr in 2012 [1]. Zhe Zhang gave some important results of this index in 2013[19]. The Merrifield index of triphenylene, Acyclic, bycyclic and tricyclic molecular graphs are calculated by Gutman, Gultekin and Sahin in 2016 [**?**]. The Merrifield-Simmons index of hexagonal structure has been studied in terms of molecular topology. In statistical mechanics, an approximately similar problem of counting the possibilities of putting particles in the sites of a 2-dimensional lattice such that no two share the same site. Now, the formal definition of Merrifield-Simmons index is as follows:

Definition 4.2.

Let $n(G, k)$ be the number of distinct k-element vertex set then the Merrifield-Simmons index is defined as

$$\sigma = \sigma(G) = \Sigma\ limits_{k \geqslant 0} n(G, k) \tag{4.4.1}$$

4.4.2 Examples

In chap 1, we have studied about the independent sets. To compute Merrifield-Simmons index, first we have to find all independent sets in a graph. The total number of independent sets is known as Merrifield-Simmons index. Let's have some examples:

Example 4.4.1. *Consider a very simple graph as shown in fig 4.1:*

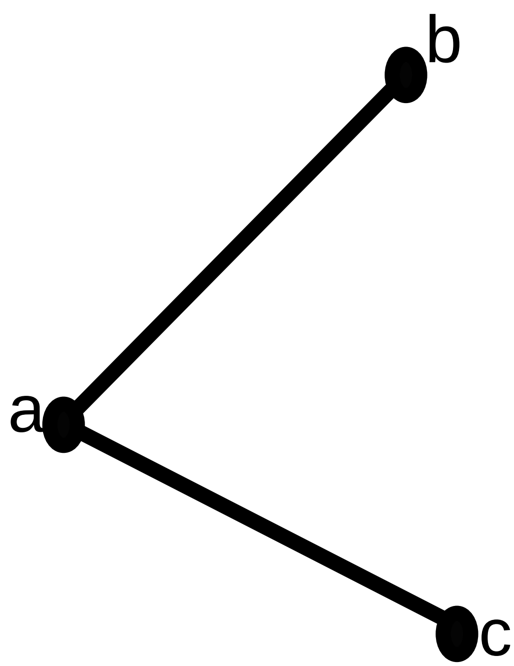

Figure 4.1: Graph H

The independent sets are as follows:

s_1={a},

s_2={b},

s_3={c} *and*

s_4={b,c}

So, there are 4 independent sets. Hence the Merrifield-Simmons index is 4.

Example 4.4.2. *Consider a very simple graph as shown in fig 4.2:*

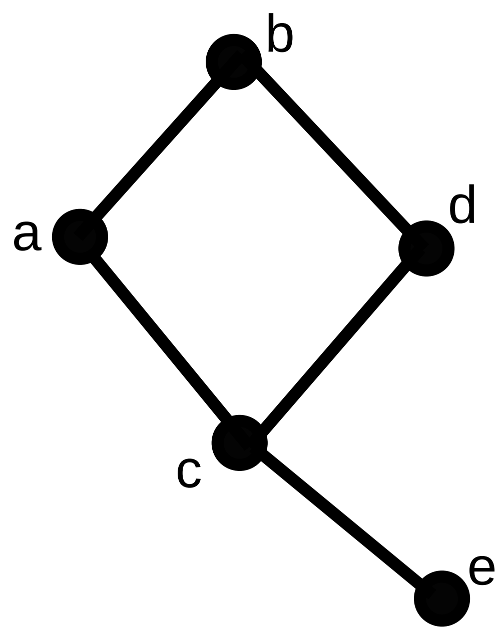

Figure 4.2: Graph H_1

The independent sets are as follows:

s_1={a},

s_2={b},

s_3={c},

$s_4 = \{d\},$

$s_5 = \{e\},$

$s_6 = \{a, e\},$

$s_7 = \{b, e\},$

$s_8 = \{d, e\},$

$s_9 = \{a, d\},$

$s_{10} = \{b, c\}\, and$

$s_{11} = \{a, d, e\}$

So, there are 11 independent sets. Hence the Merrifield-Simmons index is 11.

In next chapter, we will find Merrifield-Simmons index of V- Phenlynic nanosheet and nanotube.

Chapter 5

Merrifield-Simmons index of V-phenylenic nanosheet and nanotube

5.1 Introduction

In this Chapter we will find some results regarding Merrifield-Simmons index of nano structures. The nanostructure that is taken for this research is V- phenlynic nanosheet and nano tube. Our main problem is to find Merrifield-Simmons index of V- phenylenic nanosheet and nanotube. For this, first we have to compute independent sets by an algorithm which is developed by me. Then we make transfer matrices and at the end by multiplying our tansfer matrix with column vector, we will get the final result i.e. Merrifield-Simmons index.

5.2 Merrifield-Simmons index for V-Phenlynic nanosheet

Let *G=VPHY[p,q]* denote a nanosheet (where p and q belongs to positive integers), p represents the rows and q represents the column of nanosheet whose hexagons are line up with p(rows) and q(columns) as follows: Now we introduce some vectors of (zeroes) and (ones).

Some important results regarding computations for X_p:

Let X_p represents the vectors that can be taken as column of independent set of $G = VPHY[p, q]$. Then X_p is a selection of 2p- vectors of (zeroes) and (ones).

Theorem 5.1. *Let X_p denote the combination of all possible 2p- vectors whose entries are in the form of (zeroes) and (ones). Then the columns in (3l+1)-th & (3l+3)-th position of an independent sets are choosen from X_p, where $1 \leq l \leq q - 1$.*

Theorem 5.2. *Let X_p denote the combination of all possible 2p- vectors whose entries are in the form of (zeroes) and (ones). Then no consecutive (ones) take up the place of the (2l-1)-th & 2l-th position, where $1 \leq l \leq p$.*

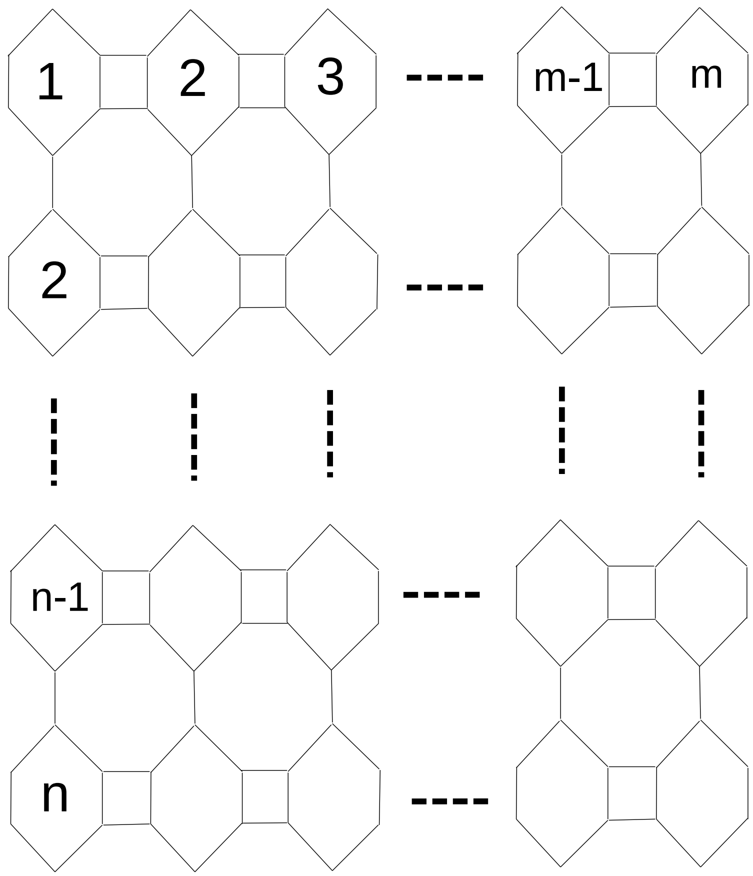

Figure 5.1: *VPHY[p,q]*

Theorem 5.3. *Let X_p denote the combination of all possible 2p- vectors whose entries are in the form of (zeroes) and (ones). The cardinality of X_p is 3^p.*

Some important results regarding computations for Y_p:

Let Y_p represents the vectors that can be taken as column of independent set of $G = VPHY[p, q]$. Then Y_p is a collection of (p+1)- vectors of (zeroes) and (ones).

Theorem 5.4. *Let Y_p denote the combination of all possible (p+1)- vectors whose entries are in the form of(zeroes) and (ones). Then the columns in (3l+2)-th position* *of an independent set is choosen from Y_p, where $0 \leq l \leq q-1$.*

Theorem 5.5. *Let Y_p denote the combination of all possible (p+1)- vectors whose entries are in the form of (zeroes) and (ones). The cardinality of Y_p is 4.3^{p-1}.*

Following is an algorithm, by which we can get some conditions regarding joining of X_p and Y_p.

5.2.1 Algorithm for nanosheet

Let *u(j)* represents a vector u which is at $j-th$ position. Thus, two column vectors u and $u^{'}$ must satisfy one of the following two conditions to become a pair of column that should be consecutive in an independent set of G if and only if,

1. u and $u^{'}$ are choosen from Y_p and X_p respectivly and they are othogonal to each other.

2. u and $u^{'}$ are choosen from X_p and they are orthogonal to each other.

Let we are gluing column u_{j+1} in the *(j + 1)-th* position to the right of column u_j in the *j-th* position as step *j.* The gluing process is as follows:
For fixing p and q, we can obtained the independent sets of G by applying gluing process which is as follows:

1. For the first column of I, select a vector against X_p and named it v.Similarly, choose a vector against Y_p and named it w. if v and w satisfy (1) then glue vector w towards the right side of v.

2. choose a vector from X_p and named it $v^{'}$. if $v^{'}$ and w satisfy (1) then glue vector $v^{'}$ towards the right side of w.

3. if $v^{'}$ and $v^{''}$ satisfy (2) then glue vector $v^{''}$ towards the right side of $v^{'}$.

Reiterate the above procedure as far as *(3q)-th* position of the column is glued.

5.2.2 Transfer Matrix

We will move forward to our computations with the help of transfer matrices as follows:

- Let B_{p_1} describes the transfer matrix for step 1. Then B_{p_1}=$(B_{v1,v2})$ is $3^p \times 4.3^{p-1}$ matrix with vectors of X_p serve as rows and vectors of Y_p serve as columns.

- In matrix B_{p_1}, access of the position (ξ, η) must be 1 if the vectors represented as ξ, η orthogonal, and 0 otherwise.

- The transfer matrix for step 2 is denoted by B_{p_2} must be the transpose of B_{p_1}.

- The transfer matrix for step 3 is denoted by $3^p \times 3^p$ matrix. It is denoted by B_{p_3} with vectors of X_p serves as the rows as well as columns.

- In matrix B_{p_3}, access of the position (α, β) must be 1 if the vectors represented as α, β orthogonal, and 0 otherwise.

Note that B_{p_1} represents the transfer matrix for each step j while $j = 3l + 1$ (where $(0 \leq l \leq q - 1)$, B_{p_2} represents the transfer matrix for every step j while $j = 3l + 2$ (where $0 \leq k \leq q - 1$) and B_{p_3} is the transfer matrix for every step j while $j = 3l + 3$

(where $0 \leq l \leq q-1$).

So,

The transfer matrix for *G=VPHY[p,q]* is

$$B_p = B_{p_1} B_{p_2} B_{p_3}$$

For Merrifield-Simmons index, we have

$$M(VPHY[p,q]) = b(p,q) = 1 \cdot B_p^q \cdot 1 \tag{5.2.1}$$

Here 1 represents the vector with all entries 1. We can say B_p is a transfer matrix with triple step because it is given as multiplication of three transfer matrices.

Example 5.2.1. *Consider a graph $G = VPHY = [1,1]$, as shown in fig 5.1*

Following are X_p and Y_p:

X_p	Y_p
(0,0)	(0,0)
(0,1)	(0,1)
(1,0)	(1,0)
	(1,1)

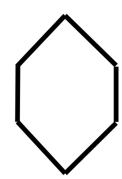

Figure 5.2: VPHY[1,1]

Then we have two transfer matrices for $G = VPHY[1,1]$ as follows: $B_{1_1} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$

,

$B_{1_2} = T_1^T = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$ *Now we multiply these transfer matrices for $G = VPHY[1,1]$ as follows:*

$$B_1 = B_{1_1} \cdot B_{1_2}$$

$$B_1 = \begin{pmatrix} 4 & 2 & 2 \\ 2 & 2 & 1 \\ 2 & 1 & 2 \end{pmatrix}$$

Now apply equation 5.2.1.

Let $M(VPHY[1,1])$ be the Merrifield-Simmons index then

$$M(VPHY[1,1]) = 18$$

Example 5.2.2. *Consider a graph $G = VPHY[2,3]$,*

Following are X_p and Y_p:

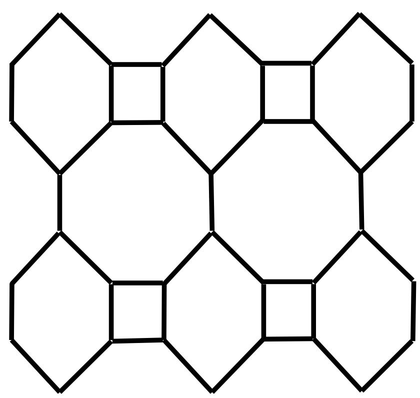

Figure 5.3: VPHY[2,3]

X_p	Y_p
(0,0,0,0)	*(0,0,0,0)*
(0,0,0,1)	*(0,0,0,1)*
(0,0,1,0)	*(0,0,1,0)*
(0,1,0,0)	*(0,1,0,0)*
(0,1,0,1)	*(0,1,0,0)*
(0,1,1,0)	*(0,1,0,1)*
(1,0,0,0)	*(1,1,0,1)*
(1,0,0,1)	*(1,0,0,0)*
(1,0,1,0)	*(1,0,0,1)*
	(1,0,1,0)
	(1,0,1,1)
	(1,1,0,0)

Then we have three transfer matrices for $G = VPHY[2,3]$ *as follows:*

$$B_{2_1} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$B_{2_2}=B_{2_1}^{T}=\begin{pmatrix} 1&1&1&1&1&1&1&1&1\\ 1&0&1&1&0&1&1&0&1\\ 1&1&0&1&1&0&1&1&0\\ 1&1&1&0&0&0&1&1&1\\ 1&0&1&0&0&0&1&0&1\\ 1&0&1&0&0&0&0&0&0\\ 1&1&1&1&1&1&0&0&0\\ 1&0&1&1&0&1&0&0&0\\ 1&1&0&1&1&0&0&0&0\\ 1&0&0&1&0&0&1&0&0\\ 1&0&0&1&0&0&0&0&0\\ 1&1&1&0&0&0&0&0&0 \end{pmatrix},$$

$$B_{2_3}=\begin{pmatrix} 1&1&1&1&1&1&1&1&1\\ 1&0&1&1&0&1&1&0&1\\ 1&1&0&1&1&0&1&1&0\\ 1&1&1&0&0&0&1&1&1\\ 1&0&1&0&0&0&1&0&1\\ 1&1&0&0&0&0&1&1&0\\ 1&1&1&1&1&1&0&0&0\\ 1&0&1&1&0&1&0&0&0\\ 1&1&0&1&1&0&0&0&0 \end{pmatrix}$$

Now we multiply these transfer matrices for G=VPHY[2,3] as follows:

$$B2 = B_{2_1} \cdot B_{2_2} \cdot B_{2_3} \cdot B_{2_1} \cdot B_{2_2} \cdot B_{2_3} \cdot B_{2_1} \cdot B_{2_2}$$

$$B_2 = \begin{pmatrix} 471120 & 283564 & 336936 & 336936 & 204572 & 202752 & 283564 & 170572 & 204572 \\ 283564 & 170950 & 202584 & 202916 & 123398 & 121936 & 170644 & 102813 & 122980 \\ 336936 & 202584 & 241224 & 240768 & 146032 & 145056 & 202916 & 121930 & 146540 \\ 336936 & 202916 & 240768 & 146032 & 146540 & 145056 & 202584 & 121930 & 146032 \\ 204572 & 123398 & 146032 & 145056 & 89162 & 88000 & 122980 & 74137 & 88560 \\ 202752 & 121936 & 145056 & 145056 & 88000 & 87360 & 121936 & 73288 & 88000 \\ 283564 & 170644 & 202916 & 202584 & 122980 & 121936 & 170950 & 102813 & 123398 \\ 170572 & 102813 & 121930 & 121930 & 74137 & 73288 & 102813 & 61934 & 74137 \\ 204572 & 122980 & 146540 & 146032 & 88560 & 88000 & 123398 & 74137 & 89162 \end{pmatrix}$$

Now apply equation 5.2.1.

Let $M(VPHY[p,q])$ be the Merrifield-Simmons index, then

$$M(VPHY[2,3]) = 13209830$$

Example 5.2.3. *Consider a graph $G = VPHY = [2,7]$,*

The matrix B after multiplying transfer matrices is as follows:

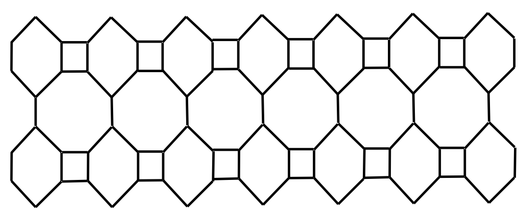

Figure 5.4: VPHY[2,3]

$$B=\begin{pmatrix}
926966125818112 & 558040720655680 & 662914415631232 & 398862705444352 & ... & 558040720655680 \\
558040720655680 & 335944804237296 & 399079556004320 & 240118407805824 & ... & 335944790843184 \\
662914415631232 & 399079556004320 & 474079386383808 & 285244336911616 & ... & 399079572457184 \\
398862705444352 & 240118407805824 & 285244336911616 & 171625968378880 & ... & 240118407805824 \\
402568794539328 & 242349513817136 & 287894712001632 & 173220653289344 & ... & 242349494427888 \\
662914415631232 & 399079572457184 & 474079366159040 & 285244336911616 & ... & 399079556004320 \\
402568794539328 & 242349494427888 & 287894735827040 & 173220653289344 & ... & 242349513817136 \\
335741738525376 & 202119104872688 & 240103744218016 & 144465749910656 & ... & 202119104872688 \\
558040720655680 & 335944790843184 & 399079572457184 & 240118407805824 & ... & 335944804237296
\end{pmatrix}$$

Now apply equation 5.2.1.

Let $M(VPHY[2,7])$ be the Merrifield-Simmons index, then

$$M(VPHY[2,7]) = 25992896874096720$$

5.2.3 Merrifield-Simmons index for V-Phenlynic nanotube

By identifying edges (r_j, r_{j+1}) with (r_j^*, r_{j+1}^*), (where $1 \leq j \leq 2p-1$). The lattice with cylindrical conditions, denoted as $H = VPHZ[p,q]$, can be obtained. The representation of nanotube is shown to be as vertical cylinder as follows.

Here we introduce a new vector Z_q.

Some important results regarding computations for Z_q:

Let Z_q represents the vectors that can be taken as column of independent set of H=VPHZ[p,q]. Then Z_q is a collection of q- vectors of (zeroes) and (ones).

Theorem 5.6. *Let Z_q denotes the combination of all possible q- vectors whose entries are in the form of (zeroes) and (ones). Then the column in (4l+1)-th and 4l-th position of an independent is choosen from Z_q, where $0 \leq l \leq p-1$ and $1 \leq l \leq q$.*

Theorem 5.7. *Let Z_q denotes the combination of all possible q- vectors whose entries are in the form of (zeroes) and (ones). Then the cardinality of Z_q is 2^q.*

As discussed in previous section for nanosheet, any independent set I of *H=VPHZ[p,q]* can be generated by the process of gluing of the vectors from Z_q and Y_{q-1}. The algorithm for nanotube is as follows:

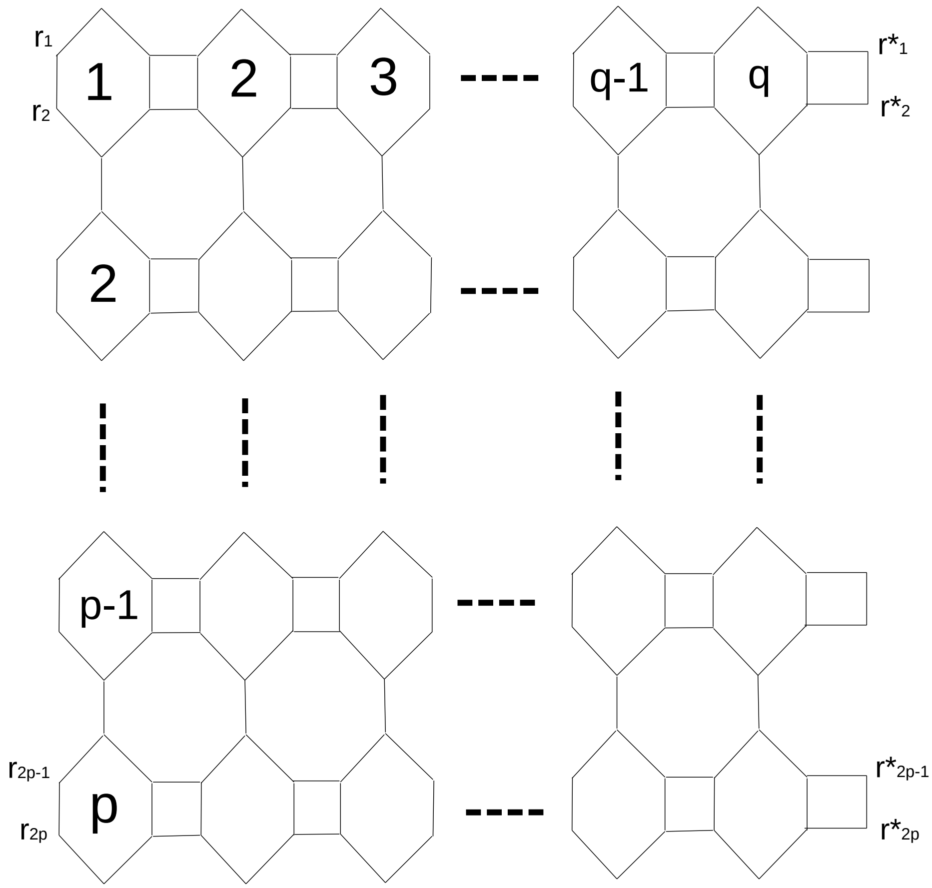

Figure 5.5: *VPHZ[p,q]*

5.2.4 Algorithm for nanotube

Following is an algorithm, by which we can get some conditions regarding joining of Z_q and Y_{q-1}. Let u represents a vector *u(j)* which is at $i-th$ position. Thus, two column vectors u and u' must satisfy one of the following two conditions to become a pair of column that should be consecutive in an independent set of $H = VPHZ[p,q]$ if and only if,

1. *u(1).u(2n)+u(1).u*$'$(1)=0 and *u(2).u*$'$(1)=0

2. $u^{'}(i).u(2i-1)$=0 and $u^{'}(i).u(2i)$=0 for i=2, 3, ..., q

Let us say the gluing process of the *(j + 1)-th* column u_{j+1} to the right of *j-th* column u_j as step *j*.

For fixed p and q, all possible independent sets I of G can be obtained by a gluing process described below.

1. Take a vector from Z_q s.t it corresponds to the first row of I, and denote it as v. Glue a vector w from Y_{q-1} to the bottom of v, such that v and w are possible consecutive vectors in I.

2. Take a vector form Y_{q-1}, denote it as $w^{'}$. Glue vector $w^{'}$ to the bottom of w such that w and $w^{'}$ are orthogonal.

3. Glue a vector $v^{'}$ to the bottom of $w^{'}$, s.t $w^{'}$ and $v^{'}$ are possible consecutive vectors in I.

4. Glue a vector $v^{''}$ to the bottom of $v^{'}$ s.t $v^{'}$ and $v^{''}$ are orthogonal.

Reiterate the above procedure as far as the *(3p+1)-th* position of the column is glued.

5.2.5 Transfer Matrix

We will move forward to our computations with the help of transfer matrices as follows:

- Let C_{q1} denote the transfer matrix for step 1. Then C_{q1} is the $2^q \times 4.3^{q-2}$ matrix with vectors of Z_q serve as rows and vectors of Y_{q-1} serve as columns.

- Let C_{q2} denote the transfer matrix for step 2. Then C_{q2} must be the $4.3^{n-2} \times 4.3^{n-2}$ matrix with vectors of Y_{q-1} serve as rows as well as columns.

- The transfer matrix for step 3 is denoted by C_{q_3} is the transpose of C_{n_1}.

- Let C_{q4} denote the transfer matrix for step 4. Then C_{q4} must be the $2^n \times 2^n$ matrix with vectors of Z_q serve as columns.

Note that C_{q_1} is the transfer matrix for every step j while $j = 4l + 1$ (where $(0 \leq l \leq p-1)$, C_{q_2} is the transfer matrix for every step j while $j = 4l+2$ (where $0 \leq l \leq p-1$), C_{q_3} is the transfer matrix for every step j while $j = 4l + 3$ (where $0 \leq l \leq p - 1$) and B_{q_4} is the transfer matrix for every step j while $j = 4l$ (where $1 \leq l \leq p$).

So,

The transfer matrix for *H=VPHZ[p,q]* is

$$C_q = C_{q_1} C_{q_2} C_{q_3} C_{q_4}$$

For Merrifield-Simmons index,

$$M(VPHZ[p,q]) = c(p,q) = 1 \cdot C_p^q \cdot 1 \tag{5.2.2}$$

where 1 represents the column vector with all entries should be 1.

Example 5.2.4. *Consider a graph H=VPHZ[2,2], as shown in fig 4.5*

Following are Z_q and Y_{q-1}:

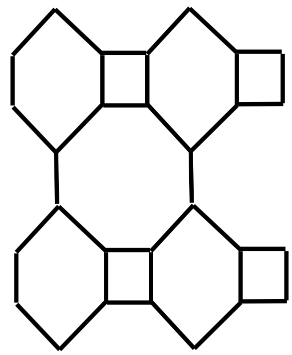

Figure 5.6: VPHZ[2,2]

Z_q	Y_{q-1}
(0,0)	(0,0,0,0)
(0,1)	(0,0,0,1)
(1,1)	(0,0,1,1)
(1,0)	(0,0,1,0)
	(0,1,0,1)
	(0,1,0,0)
	(1,1,0,0)
	(1,1,0,1)
	(1,0,1,0)
	(1,0,1,1)
	(1,0,0,1)
	(1,0,0,0)

Then we have four transfer matrices for H=VPHZ[2,2] as follows:

$$C_{2_1}=\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$C_{2_2}=\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$C_{2_3}=C_{2_1}^{T}=\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix},$$

$$C_{2_4}=\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

Now we multiply these transfer matrices for H=VPHZ[2,2] as follows:

$$C_2 = C_{2_1} \cdot C_{2_2} \cdot C_{2_3} \cdot C_{2_4} \cdot B_{2_1} \cdot B_{2_2} \cdot B_{2_3}$$

$$C_2 = \begin{pmatrix} 12981 & 5493 & 2081 & 3569 \\ 5493 & 2304 & 872 & 1501 \\ 2081 & 872 & 328 & 564 \\ 3569 & 1501 & 564 & 968 \end{pmatrix}$$

Now apply equation 5.2.2.

Let M(VPHZ[2,2]) be the Merrifield-Simmons index, then

$$M(VPHZ[2,2]) = 44741$$

Example 5.2.5. *Consider a graph H=VPHZ=[3,5], as shown in fig. 4.6*

Following are Z_q *and* Y_{q-1}*:*

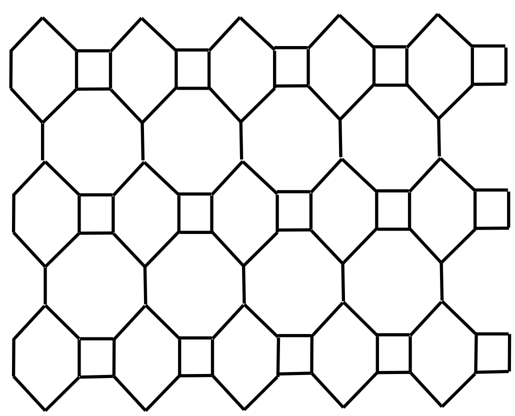

Figure 5.7: VPHZ[3,5]

Z_q	Y_{q-1}
(0,0)	*(0,0,0,0)*
(0,1)	*(0,0,0,1)*
(1,1)	*(0,0,1,1)*
(1,0)	*(0,0,1,0)*
	(0,1,0,1)
	(0,1,0,0)
	(1,1,0,0)
	(1,1,0,1)
	(1,0,1,0)
	(1,0,1,1)
	(1,0,0,1)
	(1,0,0,0)

Then we have four transfer matrices for H=VPHZ[3,5] as follows:

$$C_{5_1}=\begin{pmatrix}
1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\
1&0&0&0&0&1&1&0&0&0&0&1&1&0&0&0&0&1&1&0&0&0&0&1&1&0&0&0&0&1&1&0&0&0&0&1\\
1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1\\
1&1&1&1&0&0&0&0&0&0&0&0&0&0&1&1&1&1&1&1&1&1&0&0&0&0&0&0&0&0&0&0&1&1&1&1\\
1&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&0&0&1&1&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&1&0&1&1&0&1&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0
\end{pmatrix}$$

$$C_{5_2} = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\
1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 0 & 0 & 0 & 0
\end{pmatrix}$$

$$C_{5_3}=\begin{pmatrix}
1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\
1&0&0&1&0&1&1&0&1&0&0&1&1&0&1&0&0&1&1&0&0&1&0&1&1&0&0&1&0&1&1&0&1&0&0&1\\
1&0&0&0&0&1&1&0&0&0&0&1&1&0&0&0&0&1&1&0&0&0&0&1&1&0&0&0&0&1&1&0&0&0&0&1\\
1&1&0&0&1&1&1&1&0&0&1&1&1&1&0&0&1&1&1&1&0&0&1&1&1&1&0&0&1&1&1&1&0&0&1&1\\
1&0&0&1&0&0&0&0&1&0&0&1&0&0&1&0&0&1&1&0&0&1&0&0&1&0&0&1&0&0&0&0&1&0&0&1\\
1&1&1&1&0&0&0&0&1&1&1&1&0&0&1&1&1&1&1&1&1&1&0&0&1&1&1&1&0&0&0&0&1&1&1&1\\
1&1&1&1&0&0&0&0&0&0&0&0&0&0&1&1&1&1&1&1&1&1&0&0&0&0&0&0&0&0&0&0&1&1&1&1\\
1&0&0&1&0&0&0&0&0&0&0&0&0&0&1&0&0&1&1&0&0&1&0&0&0&0&0&0&0&0&0&0&1&0&0&1\\
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1&0&0&0&0&1&0&0&0&0&0&0&1&0&0&0&0&1&1&0&0&0&0&1&0&0&0&0&0&0&1&0&0&0&0&1\\
1&0&0&1&0&1&0&0&0&0&0&0&1&0&1&0&0&1&1&0&0&1&0&1&0&0&0&0&0&0&1&0&1&0&0&1\\
1&1&1&1&1&1&0&0&0&0&0&0&1&1&1&1&1&1&1&1&1&1&1&1&0&0&0&0&0&0&1&1&1&1&1&1\\
1&1&1&1&0&0&0&0&1&1&1&1&0&0&0&0&0&0&0&0&0&0&0&0&1&1&1&1&0&0&0&0&1&1&1&1\\
1&0&0&1&0&0&0&0&1&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&1&0&0&0&0&1&0&0&1\\
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1&0&0&1&0&1&1&0&1&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&1&0&1&1&0&1&0&0&1\\
1&1&1&1&1&1&1&1&1&1&1&1&0&0&0&0&0&0&0&0&0&0&0&0&1&1&1&1&1&1&1&1&1&1&1&1\\
1&1&1&1&1&1&1&1&1&1&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
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1&0&0&0&0&1&1&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&1&0&0&1&1&1&1&0&0&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&1&0&0&0&0&1&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
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1&0&0&1&0&1&0&0&0&0&0&0&1&0&1&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&0&0&1&0&0&0&0&0&0&1&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&1&0&0&1&1&0&0&0&0&0&0&1&1&0&0&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
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1&0&0&1&0&0&0&0&1&0&0&1&0&0&1&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&1&0&0&1&1&1&1&0&0&1&1&1&1&0&0&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&0&0&1&1&0&0&0&0&1&1&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&1&0&1&1&0&1&0&0&1&1&0&1&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0
\end{pmatrix},\ C_{5_4}=\begin{pmatrix}
1&1&1&1&1&1&1&1\\
1&0&0&1&1&0&0&1\\
1&0&0&0&0&0&0&1\\
1&1&0&0&0&0&1&1\\
1&1&0&0&0&0&0&0\\
1&0&0&0&0&0&0&0\\
1&0&0&1&0&0&0&0\\
1&1&1&1&0&0&0&0
\end{pmatrix}$$

Now we multiply these transfer matrices for H=VPHZ[3,5] as follows:

$$C_5 = \begin{pmatrix} 25440340584242768 & 10851052430962208 & 4436720057659059 & 12728381740093040 & \ldots & 7011572230477069 \\ 10851052430962210 & 4628289678272922 & 1892391086136501 & 5429031188175267 & \ldots & 2990639225778767 \\ 4436720057659059 & 1892391086136501 & 773750791646436 & 2219792341780893 & \ldots & 1222797176988858 \\ 12728381740093040 & 5429031188175267 & 2219792341780893 & 6368296923879873 & \ldots & 3508051256881023 \\ 2859541166648737 & 1219677903457132 & 498695459657670 & 1430693890559817 & \ldots & 788113330691923 \\ 1681751812678233 & 717316135536476 & 293292486084605 & 841419079376619 & \ldots & 463504649738750 \\ 5000181574463751 & 2132722161037645 & 872016621170296 & 2501706606607193 & \ldots & 1378090494336790 \\ 7011572230477069 & 2990639225778767 & 1222797176988858 & 3508051256881023 & \ldots & 1932446605676540 \end{pmatrix}$$

Now apply equation 5.2.2.

Let M(VPHZ[3,5]) be the Merrifield-Simmons index, then

$$M(VPHZ[3,5]) = 192659983888509856$$

Table 1 Merrifiled-Simmons index for $G = VPHY[p, q]$

q	b(1,q)	b(2,q)	b(3,q)
1	18	299	4957
2	274	62717	14315333
3	4182	13209830	41582131919
4	63826	2782187074	120776634724013
5	974118	585970545236	350799920160330048
6	14867074	123414229088792	1018910504691312230400
7	226902582	25992896874096720	2959460813795655887618048
8	3463007026	5474495873534007296	8595856326730098140516450304

q	b(4,q)	b(5,q)
1	82176	1362293
2	3267368264	745751961611
3	130886561875907	411986508646985920
4	5242717860955852800	227577680310235293548544
5	209999548588701121511424	125712031061214476880316465152
6	8411631287957429947256012800	69442286343623089580525026703048704
7	336931871715176640689160572633088	38359344724475782052580701646225332502528
8	13495965561036932583183101065795993600	21189384813308923969108003498501593888601407488

Table 2 Merrifield-Simmons index of $H = VPHZ[p, q]$

q	c(1,q)	c(2,q)	c(3,q)
1	14	228	3516
2	299	44741	9594706
3	4957	8749709	26080008775
4	82176	1710981072	70884301162719
5	1362293	334576864927	192659983888509856
6	22583749	65425430301589	523640162913339637760
7	374387682	12793732542561372	1423227667986599718682624
8	6206504351	2501773264784808960	3868261333273480593789681664

q	c(4,q)	c(5,q)
1	53628	818508
2	2018662416	425189027472
3	75637003320817	219710981483797760
4	366850033238310	2833797641170208768
5	106170155083700342095872	113522945075491108814848
6	3977736784754133401014894592	30307183059816087734404325450973184
7	149028603032737532295931796389888	15659450524569024215274682218528569819136
8	5583457559448240505642012533854306304	8091098081582659753212187523159595972154097664

5.3 Concluding Remarks

In this chapter, we considered nanosheet and nanotube of V- phenlynic and studies Merrifield- Simmons index. By finding the inpedependent sets we have computed Merrifield- Simmons index of V- Phenlynic nanosheet and nanotube. We developed some algorithms to compute number of independent sets. We developed matlab program of the algorithms to complete our computations. We have computed Merrified-Simmon index of nanosheet and nanotube of V- phenlynic.

Chapter 6

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