Topological Description of Mobius Strip via Degree Based Indices

MS Thesis

by

MAIRA RIAZ

CIIT/SP22-RMT-016/LHR

COMSATS University Islamabad, Lahore Campus. Pakistan

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A thesis submitted to
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In partial fulfillment
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Master of Science
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by
Maira Riaz

CIIT/SP22-RMT-016/LHR

Department of Mathematics
Faculty of Science

COMSATS University Islamabad, Lahore Campus
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Maira Riaz	Registration Number
Maira Riaz	CIIT/SP22-RMT-016/LHR

Supervisory Committee

Supervisor Dr. Hani Shaker Associate Professor Department of Mathematiccs COMSATS University Islamabad (CUI) Lahore Campus	**Member** Dr. Associate Professor Department of Mathematiccs COMSATS University Islamabad (CUI) Lahore Campus
Member Name Associate Professor Department of Mathematiccs COMSATS University Islamabad (CUI) Lahore Campus	**Member** Dr. Associate Professor Department of Mathematiccs COMSATS University Islamabad (CUI) Lahore Campus

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Maira Riaz

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Has been approved

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External Examiner:____

Dr. External Examinor

University Name

Supervisor:____

Dr.

Department of Mathematics, (CUI) Lahore Campus

Head of Department:____

Prof.

Department of Mathematics, (CUI) Lahore Campus

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Date:______________

Supervisor

____

Dr. Hani Shaker
Associate Professor,
Mathematics,
COMSATS University Islamabad
Lahore Campus

Dedication

To My Parents and All Family

Your unwavering love, endless support, and boundless encouragement have been my guiding lights throughout my academic journey. This thesis is a testament to the sacrifices you've made and the belief you've instilled in me. Thank you for being my pillars of strength. This achievement is as much yours as it is mine.

Acknowledgements

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

First and foremost, I would like to thank ALLAH Almighty (the most beneficent and most merciful) for giving me the strength, knowledge, ability and opportunity to undertake this research study and to preserve and complete it satisfactorily. Without countless blessing of ALLAH Almighty, this achievement would not have been possible. May His peace and blessings be upon His messenger Hazrat Muhammad (PBUH), upon his family, companions and whoever follows him. My insightful gratitude to Hazrat Muhammad (PBUH) Who is forever a track of guidance and knowledge for humanity as a whole. In my journey towards this degree, I have found a teacher, an inspiration, a role model and a pillar of support in my life, my kind.

Maira Riaz
CIIT/SP22-RMT-016/LHR

Abstract

Topological Description of Mobius Strip via Degree Based Indices

By

Maira Riaz

Scientists study tiny building blocks called molecules. These molecules have shapes and patterns, and scientists use something called molecular graph theory to understand them. They also use special math formulas called topological indices. In our project we looked at a special shape called Hexagonal Mobius strip. It's like a twisted cylinder with loop on one side, and it can be big or small. It comes in variety of sizes and shapes and while some Mobius strip are simple to picture in regular space, few are more difficult. We wanted to know two things: how molecules act (heat of formation/entropy) and the structure of molecules (topological indices and co indices). To figure this out, we used a method called Curve Fitting on the Hexagonal Mobius strip.

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Chapter 1
Introduction

The model of graph theory announced by Swiss Mathematician leonhard Euler in 1736 by a famous example ”Seven Bridges of Königsberg problem,” is regarded as the origin of graph theory. Euler wondered if you could walk around the city, crossing each bridge only once. To crack this riddle, Euler turned it into a math concept, creating what we now call a ”Graph”. That graph provided a straightforward representation of city’s layout and bridges. Euler’s innovative approach in tackling this problem marked the birth of graph theory, a branch of math that explores connections and relationships using diagrams. This innovative idea starts a new field that,s useful in many different ways. Graphs are like pictures that help us see how things are connected. We use them to understand relationships and patterns in different fields like biochemistry, electrical engineering, computer science, transportation and operation research. The Graph theory is like a special part of math that studies graph and what they can tell us. It help us figure out the different shapes and patterns in all kind of graphs. By using this, we can solve problems about network, relationships ans systems that are linked together.

Chemical graph theory is the topology branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena. So, it’s like drawing a map of molecules to see how the different parts are connected. The concept of chemical graph is a labelled graph whose vertices corresponding to the atoms of the compound and edges corresponding to chemical bonds. This way, scientists can learn more about the shape and qualities of chemicals. This helps in various things like designing new drugs or understanding how different molecules behave. Chemical graph theory derived topological indices can be used to model the geometric structure of chemical substances. Chemical graph theory started when people started using a math idea called ”graph theory” in the late 1800s. Mathematicians like Leonhard Euler and Arthur Cayley helped create this idea. Graph theory became a helpful way to show the shapes of molecules in a formal and organized manner. With the rise of computational chemistry, using graph theory to understand how molecules are put together and predict how they act became more advanced. Now, scientists often use computer programs and special math techniques to study the structures of molecules and how chemicals react with each other.

A structural physicochemical properties of a molecule or part of a molecule is known as a molecular descriptor. They are important in studying how chemicals work and help in study the relationship between structure and properties of chemical. There are two main types of descriptors: topological indices and counting polynomials. Topological indices give information about the atoms are connected in a molecule, and they have become very popular in recent years. We can use these descriptors to studies to predict the properties of chemicals without actually making them first.

This thesis arranged in the following way:

In Chapter 2, explained some simple ideas about graphs that are important for understanding the thesis and also introduced the terms that will be used in the following chapters. This helps to followalong better as we explore more complex concepts. So, it's like setting the stage for what comes next in the thesis.

In Chapter 3 focuses on exploring chemical graph theory. In this chapter, look into things like degree based topological indices and co indices. We are also going to dive into entropy, which is a concept related to these indices and co indices. Entropy helps use to figure out how much disorder or randomness is in the molecule's structure.

The Mobius strip is a mathematical object that seems like a loop but has a twist. We can find it interesting because it's great for explaining topology, a part of math dealing with shapes and spaces. This strip is famous for showing how a tiny change can make super exciting. It's simple thing with surprising math behind it. It can make your brain think differently about math. The Mobius strip also used in art and design. The conveyor belt's duration rises in a high valume facility by constructing it as a Mobius strip. Artists and teachers like to use it to show ideas about infinity, symmetry and something called non-orientability. Mobius strip helps to see and understand things in art and design in a really intersting way. Now, think of a Mobius strip like a twisted ribbon with a loop on one side. What's cool is that it seems to have two sides, but it's really just one continuous side. This makes Mobius strip special in shape. The Mobius strip's journey from its discovery in the

19th century to its current status as an iconic mathematical object highlights its significance in both mathematical exploration and its cultural impact.

Chapter 4 focuses entirely on the most important finding. We investigate particular measures, like topological indices and co indices, for our special graph known as the Mobius strip. Then we examine how much these measures can change, which we call entropy. The main idea is connecting the topological indices to their entropies and likewise for co indices and their entropies. Furthermore, we explore how these measures are linked to the heat of formation usinga method called curve fitting. This method helps us to see how different things are connected in a clear and straightforword way. In simple words, we are figuring out special values for our graph and seeing how they relate to each other. We are using these measures to making things easier to understand for everyone interested in our research.

In Chapter 5, shared the final thoughts or wrap up everything. We talk about what we learned. We share our final thoughts and sum up all the important things we measured. It's putting together the main ideas and making a conclusion about everything we discovered.

Chapter 2
Basic Concepts

2.1 Introduction:

This chapter is all about the key ideas in graph theory. These ideas are super important to make a good base for the rest of study.

2.2 Basic Elements for Graph Theory:

In this part, we give an official explanation about graph and talk about the different words we used to describe its parts.

Definition 2.2.1. Let $G = (V, E)$ made up of a set of nodes, known as vertices (V), and lines, known as edges (E) that connect with pairs of vertices. The study of graph, which are mathematical structure which represent relationship between objects pairwise is known as graph theory.

Definition 2.2.2. The order of a graph is how many vertices it has, and the size of a graph is how many edges that graph has.

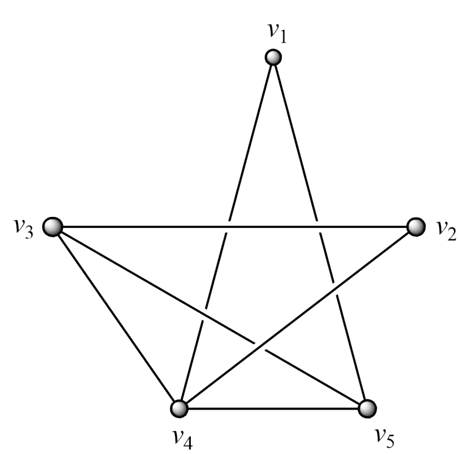


Figure 2.1: Graph

For the given example,the vertex set and the edge set are;

$$\begin{aligned} V(G) &= \{v_1, v_2, v_3, v_4, v_5\} \\ E(G) &= \{v_1v_4, v_1v_5, v_2v_4, v_2v_3, v_3v_5, v_3v_4, v_4v_5\} \end{aligned}$$

There are 5 vertices in total and there are 7 edges connecting them. So, we can say that the size of graph is 5 (because there are 5 vertices) and the order of graph is 7 (because there are 7 vertices).

Definition 2.2.3. The vertices in simple graphs are connected by single edge and there are no loop or multiple edges between vertices.

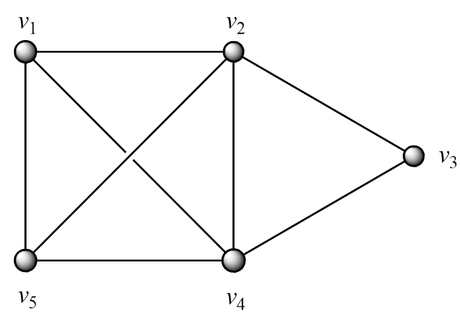


Figure 2.2: Simple Graph

Definition 2.2.4. The vertices in multiple graphs are connected by multiple edges and there can also be loops in graphs.

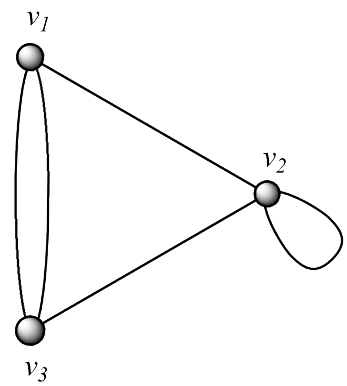


Figure 2.3: Multiple Graph

The 2.2, we can clearly see that there is no loop and every two vertex connected with single edge, this make the graph simple. But in the other 2.3, the vertex v_2 has a loop and also vertex v_1 and v_3 connected with more then one vertex, this means the graph in 2.3 is multiple graph.

Definition 2.2.5. A connected graph, every pair of vertices in a graph is connected if there is a path connecting them.

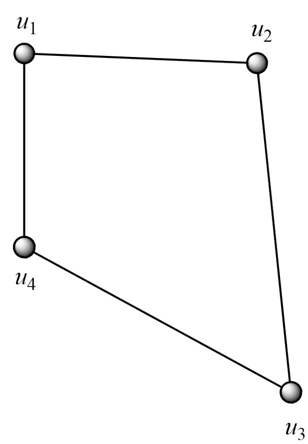


Figure 2.4: Connected Graph

Definition 2.2.6. A disconnected graph, not every pair of vertices in the graph has a path connecting them.

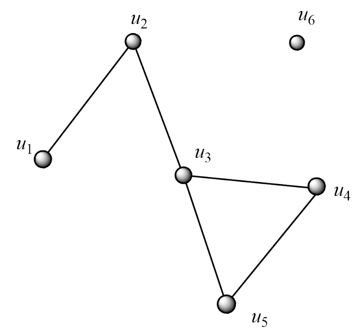


Figure 2.5: Disconnected Graph

In 2.4, each pair of vertices is connected by at least one path, this implying that the vertices are interconnected. But in 2.5, a vertex u_6 lacks connections to other vertices, it indicates that there is no path or link between this vertex and any other vertices. That's mean 2.5 is disconnected graph.

Definition 2.2.7. A graph in which there is an edge connecting each pair of unique vertices is said to be complete.

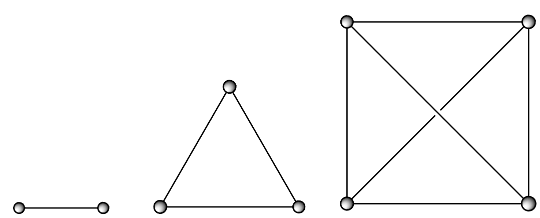


Figure 2.6: Complete Graph

Definition 2.2.8. A graph in which there is not an edge connecting each pair of unique vertices is said to be incomplete.

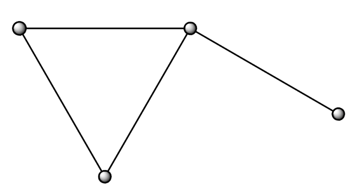


Figure 2.7: Incomplete Graph

Fig 2.6, every vertex of graph connecting with each other with an edge. In fig 2.7, some vertices are not connecting with each other.

Definition 2.2.9. Every vertex in a regular graph connecting with same number of edges, or every vertex has equal degree.

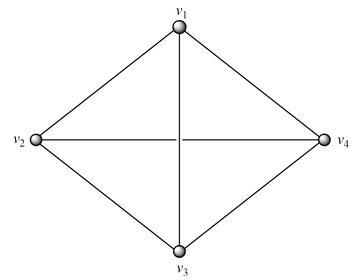


Figure 2.8: Regular Graph

Definition 2.2.10. Every vertex in a irregular graph connecting with different number of edges, or every vertex has different degree.

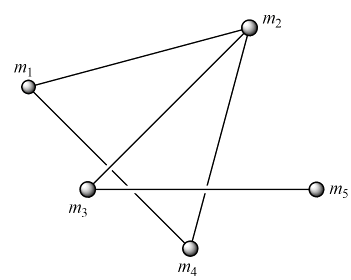


Figure 2.9: Irregular Graph

Every vertex of graph of fig 2.8 have equal degree 3 which means that graph is 3 regular graph. But in the graph of fig 2.9 degree of $m_1 = 2$, degree of $m_2 = 3$, degree of $m_3 = 2$, degree of $m_4 = 2$ and degree of $m_5 = 1$. We can clearly see that every vertex has different degree which means its an irregular graph.

Definition 2.2.11. In a graph, a walk means to going from one vertex to another vertex by following the edges. Length of the walk is the total number of edges which are covered in a walk.

Definition 2.2.12. In a graph, a path is a walk in which all the vertices are distinct, which means you can't choose to follow the same vertex more than one.

Definition 2.2.13. A cycle is a closed path that starts and ends at the same vertex.

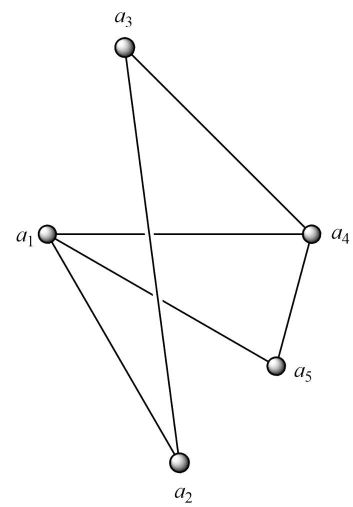


Figure 2.10: Cycle

Here i mention below walk, path and cycle from the graph in 2.10.

Walk $(a_1 - a_4 - a_5 - a_1 - a_2 - a_3)$

Path $(a_1 - a_2 - a_3 - a_4 - a_5), (a_1 - a_5 - a_4 - a_3)$

Cycle $(a_1 - a_2 - a_3 - a_4 - a_5 - a_1)$

Definition 2.2.14. A cyclic graph is a unique type of graph which contains at least one cycle.

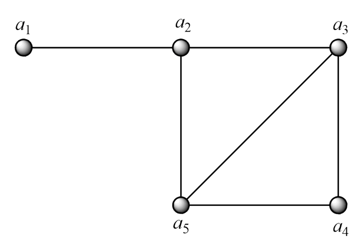


Figure 2.11: Cyclic Graph

The graph in 2.11 is a cyclic graph because it has cycles in it. Some are listed below:

$$a_2 - a_3 - a_4 - a_5 - a_2$$

$$a_2 - a_3 - a_5 - a_2$$

$$a_3 - a_4 - a_5 - a_3$$

Definition 2.2.15. Distance in a graph is all about to find out number of edges you have to cross when taking the shortest path between two vertices.

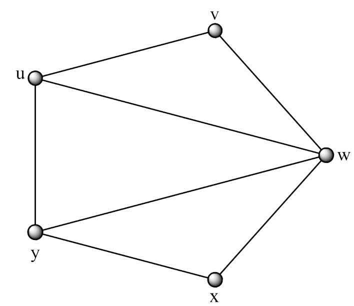


Figure 2.12: Distance in Graph

The distance between u and x is $d(u,x) = 2$ because the shortest path between them is $u - v - x$.

Chapter 3
Chemical Graph Theory

3.1 Introduction

In this chapter, we explore the structure of our graph which is Mobius strip and delve into topics like topological indices and topological co indices. We discuss how these concepts help us understand the unique properties and connections within the graph in a simple way.

3.2 Structure of Mobius Strip

An interesting mathematical object known as the Mobius strip was discovered in 1858 by two German Mathematicians J. B. Listing and A. F. Mobius. Imagine you have a long, flat ribbon. Now twist one side of the ribbon around by 180 degree and then connect the both ends of the ribbon together. The hexagonal Mobius strip is a unique shape which is resembling with a twisted ribbon who featuring six sides. The Mobius strip is a fascinating math object that looks like a long, flat ribbon but with a twist in the middle. An authentic substance Mobius strips are inflexible material that, when left to itself, take on a unique form that is not dependent to the type of material. So, if you follow along its surface, you go on both the inside and outside without any break. This is how a Mobius strip made [1]. Mobius strip used a lot in different technical fields and research.Even though they can look different in shaps and sizes, most of them exist in regular three-dimensional space. They are special because of their topology, which means they have endless nature. Mobius strip often used to show students ideas about topology and geometry. Compared to a regular cylindrical shape, a mobius strip has double the number of edges on its boundary, even though both have the same avarage diameter. this makes the Mobius strip better because it has a longer path.

The Mobius strip is a special shape that scientists use in different areas of science. The Mobius strip exists in the real world as a physical object. It has been used as an imagery

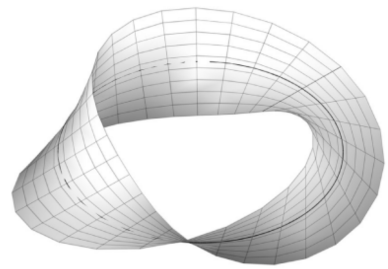
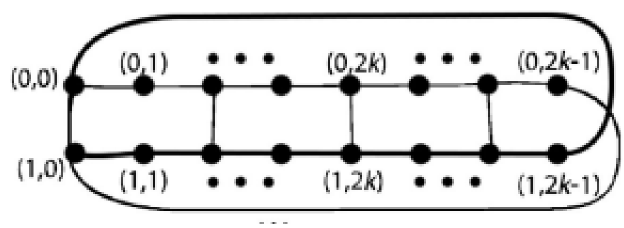
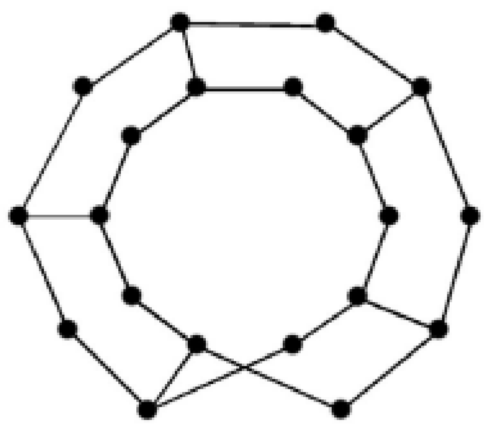


Figure 3.1: Mobius Strip



(a): HM_n



(b): HM_5

Figure 3.2: Chemical structure of Hexagonal Mobius Strip

tool to clarify ideas like of one-sided object and non-orientability. Another interesting use is in electromagnetic resonators and filters. It acts like a special electromagnetic strip that vibrates at half the frequencies of a regular electromagnetic cylinder. The Mobius strip is unique shape that works well for certain electromagnetic uses [2]. In the world of communication tech, there is something cool called Mobius strip resonators. They do not resemble the typical devices employed for various frequency bands. Unlike regular devices for different frequencies, these resonators help us make compact and powerfull oscillators that can workin many frequency bands. This leads to smaller and better communication gadgets in the end [3].

3.3 Chemical Graph Theory

In a chemical graph, vertices (atoms) and edges (bonds) show how atoms are in chemical molecule put together. The edges tells us how atoms are linked by bonds, each vertex is like a symbol an atom, It's kind a map that helps us see the atoms and bonds in a chemical molecule. The branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical activities . Chemical graph theory, a part of chemistry, brings together graph theory and chemistry [10, 11]. It's like using a secret code to explore and understand the complicated world of molecules and how they interact with each other.

3.4 Topological Indices

We can discover things about chemicals using a special number called a topological index, which was Wiener's discovery. A topological index is a molecular structure descriptor calculated from a molecular graph of a chemical compound which characterizes its topology. Various topological indices are categorized based on their degree, distance and spectrum. This number helps us understand how a chemical structure is connects to its properties, such as how it interact with living things, reacts with other stuff, and changes things like boiling points. Topological indices in chemistry include processing information, uniqueness determination, isomer generation and prediction of neuclear magnetic resonance spectra. Topological indices are usually used for quantitative-structure property relationships (QSPR) and quantitative structure action relationships (QSAR). They look at the structure of the chemical and how atoms are linked without getting into details about the types of atoms or their bonding. Understanding the biological effects of a chemical require an understanding of this simple method. It allows us to spot patterns and connections between structure of chemicals and its function in living things. In simple words, How topological indices help us uncover the mysteries of how a chemical affects o a living organisms by paying attention to its structure and connection [4].

Topological indices have two types; 1. Degree Based Topological indices 2. Distance

Based Topological indices. Here we talk about somee degree based topological indices below in table 3.1.

Table 3.1: Degree Based Topological Indices

Topological Indices	Functions
1^{st}, 2^{nd} and 3^{rd} Redefine Zagreb index [5]	$\begin{aligned} ReZG_1(G) &= \sum_{st\in G}\left(\frac{\alpha(s)+\alpha(t)}{\alpha(s)\times\alpha(t)}\right) \\ ReZG_2(G) &= \sum_{st\in G}\left(\frac{\alpha(s)\times\alpha(t)}{\alpha(s)+\alpha(t)}\right) \\ ReZG_3(G) &= \sum_{st\in G}((\alpha(s)+\alpha(t)) \\ &\times ((\alpha(s)\times\alpha(t)) \end{aligned}$
1^{st} and 2^{nd} K Banhatti index [6]	$\begin{aligned} B_1(G) &= \sum_{st\in G}(\alpha(s)+\alpha(t)) \\ B_2(G) &= \sum_{st\in G}(\alpha(s)\times\alpha(t)) \end{aligned}$
1^{st} and 2^{nd} Modified K Banhatti index [7]	$\begin{aligned} MB_1(G) &= \sum_{st\in G}\frac{1}{\alpha(s)+\alpha(t)} \\ MB_2(G) &= \sum_{st\in G}\frac{1}{\alpha(s)\times\alpha(t)} \end{aligned}$
1^{st} and 2^{nd} Hyper K Banhatti index [8]	$\begin{aligned} HB_1(G) &= \sum_{st\in G}(\alpha(s)+\alpha(t))^2 \\ HB_2(G) &= \sum_{st\in G}(\alpha(s)\times\alpha(t))^2 \end{aligned}$
sum connectivity index [8, 9]	$SB(G) = \sum_{st\in G}\frac{1}{\sqrt{\alpha(s)+\alpha(t)}}$

3.5 Topological Co-indices

Topological co-indices are a way to study molecular shapes by considering both the mathematical representation of molecules and their physical properties. In simple words, topological co index is a mathematical formula that can be applied to any graph which models some molecular structure. These co indices are computed for non-adjacent pair of vertices. We can use these co indices to speed up our research. The calculation of these topological co indices offers scientists to quickly identify particular characteristics of molecules without having to spend a lot of time performing laborious experiments in the laboratories. Topological co indices are like a quick track for scientists to learn how molecules act without doing long experiments and help researchers quickly get insights into the properties and behavior of molecules, making the study of chemistry easier and faster [12]. Here some topological co indices which we determine, mention below in table 3.2.

3.6 Entropy

Entropy [23], an idea from scientist Shannon [24], helps us to understand how a system gets really unpredictable when it can't go back to where it began. Another researcher Dehmer [25, 26], is looking into these entropies to understand and use them better. More authore have also looked at the entropy of topological indices. In chemistry, information entropy is now used in two modes. First one is, it is a structural descriptor for assessing the complexity of chemical structures. second one is, informatiom entropy s usefull in this regard for connecting structural and physico chemical features numerically distinguishing isomers of organic molecules and classifying natural products and synthetic chemicals. Adding to what we know in this field [27, 28, 29, 30]. The general form of entropy is following,

$$\begin{aligned} E(G) &= -\sum_{k=1}^{n}\left(\frac{\alpha(a(s)_k a(t)_k)}{T}\right) log\left(\frac{\phi(a(s)a(t))}{T}\right) \\ &= log(T) - \frac{1}{T}\sum_{k=1}^{n} I_k \alpha(a(s)_k a(t)_k) log \alpha(a(s)_k a(t)_k) \end{aligned}$$

Table 3.2: Degree Based Topological Indices

Topological co-Indices	Functions
1^{st} and 2^{nd} Zagreb co-index [13, 14, 15, 16, 17]	$\overline{M_1(G)} = \sum_{st\in G}(\alpha(s)+\alpha(t))$ $\overline{M_2(G)} = \sum_{st\in G}(\alpha(s)\times\alpha(t))$
Randic co-index [18, 19]	$\overline{R_\beta}(HM_n) = \sum_{st\in HM_n}(\alpha(s)\times\alpha(t))^\beta$ $\beta = (\frac{-1}{2},-1,1,\frac{1}{2})$
Forgotten co-index [20]	$\overline{F(G)} = \sum_{st\in G}(\alpha(s)^2+\alpha(t)^2)$
Hyper Zagreb co-index [21]	$\overline{HM(G)} = \sum_{st\in G}(\alpha(s)+\alpha(t))^2$
1^{st} and 2^{nd} Multiple Zagreb co-index [22]	$\overline{PM_1(G)} = \prod_{st\in G}(\alpha(s)+\alpha(t))$ $\overline{PM_2(G)} = \prod_{st\in G}(\alpha(s)\times\alpha(t))$

Where "$T = \sum_{k=1}^{n} I_k\alpha(a(s)_k a(t)_k)$" is a molecular index and "n" stands for the number of sets of edges. "I_k" representd the frequency, and "$\alpha(st)$" indicates the weight of an edge connecting points.

In this chapter, we discuss topological indices and co indices. Moving forward to the next chapter, we unveil the key findings and main results related to these indices.

Chapter 4
Degree-Based Topological Description of Hexagonal Mobius Strip

4.1 Introduction

This chapter focuses on unveiling our primary findings regarding topological indices, co indices and the entropy associated with these measures. Additionally, we explore these indices through curve fitting techniques. Here, we present the main results derives from our exploration in these areas.

4.2 Essential Result for Topological Invariant

We'll examine mathematical formulas related to the mentioned indices which are mentioned in Chapter 2.
Here's edge-partitioning mention below for Hexagonal Mobius Strip.

Table 4.1: Edges calculating for HM_n

$[n]$	3	4	5	6	...	n
$Vertices$	12	16	20	24	...	$4n$

Table 4.2: Edges calculating for HM_n

$[n]$	3	4	5	6	...	n
Edges	15	20	25	30	...	$5n$

Table 4.3: Edge-Partitioning of HM_n

$Frequency$	degree of edges	$(\alpha(s), \alpha(t))$
$4n$	3	$(2,3)$
n	4	$(3,3)$

Theorem 4.2.1. *The first, second and third Zagreb index for $G = HM_n$, $n \geq 3$ is given by $ReZG_1(HM_n) = 4n$, $ReZG_2(HM_n) = 6.3n$ & $ReZG_3(HM_n) = 174n$.*

Proof:

By using Table 3.1 for $ReZG_1(HM_n)$, $ReZG_2(HM_n)$ and $ReZG_3(HM_n)$ and Table 4.3, we get

$$\begin{aligned}
ReZG_1(HM_n) &= \sum_{st\in G}\left(\frac{\alpha(s)+\alpha(t)}{\alpha(s)\times\alpha(t)}\right)\\
&= 4n\frac{(2+3)}{(2\times 3)}+4n\frac{(3+3)}{(3\times 3)}\\
ReZG_1(HM_n) &= 4n\\
ReZG_2(HM_n) &= \sum_{st\in G}\left(\frac{\alpha(s)\times\alpha(t)}{\alpha(s)+\alpha(t)}\right)\\
&= 4n\frac{(2\times 3)}{(2+3)}+4n\frac{(3\times 3)}{(3+3)}\\
ReZG_2(HM_n) &= 6.3n.\\
ReZG_3(HM_n) &= \sum_{st\in G}((\alpha(s)+\alpha(t))\times((\alpha(s)\times\alpha(t))\\
&= 4n((2\times 3)\times(2+3))+n((3\times 3)\times(3+3))\\
ReZG_3(HM_n) &= 174n.
\end{aligned}$$

Theorem 4.2.2. *The first and second K Banhatti Index for $G = HM_n$, $n \geq 3$ is given by $B_1(HM_n) = 58n$ & $B_2(HM_n) = 84n$.*

Proof:

Using Table 3.1 for $B_1(HM_n)$ and $B_2(HM_n)$ and Table 4.3, we obtain

$$\begin{aligned}
B_1(HM_n) &= \sum_{st\in G}(\alpha(s)+\alpha(t))\\
&= 4n((2+3)+(3+3))+n((3+4)+(3+4))\\
B_1(HM_n) &= 58n.\\
B_2(HM_n) &= \sum_{st\in G}(\alpha(s)\times\alpha(t))\\
&= 4n((2\times 3)+(3\times 3))+n((3\times 4)+(3\times 4))\\
B_2(HM_n) &= 84n.
\end{aligned}$$

Theorem 4.2.3. *The first and second Modified K Banhatti Index for $G = HM_n$, $n \geq 3$ is given by $MB_1(HM_n) = \frac{67}{154}n$ & $MB_2(HM_n) = \frac{37}{120}n$.*

Proof:

With the help of Table 3.1 for $MB_1(HM_n)$ and $MB_2(HM_n)$ and Table 4.3, we achieve

$$\begin{aligned}
MB_1(HM_n) &= \sum_{st\in G}\left(\frac{1}{\alpha(s)+\alpha(t)}\right) \\
&= 4n\left(\frac{1}{(2+3)+(3+3)}\right)+n\left(\frac{1}{(3+4)+(3+4)}\right) \\
MB_1(HM_n) &= \frac{67}{154}n. \\
MB_2(HM_n) &= \sum_{st\in G}\left(\frac{1}{\alpha(s)\times\alpha(t)}\right) \\
&= 4n\left(\frac{1}{(2\times 3)+(3\times 3)}\right)+n\left(\frac{1}{(3\times 4)+(3\times 4)}\right) \\
MB_2(HM_n) &= \frac{37}{120}n.
\end{aligned}$$

Theorem 4.2.4. *The first and second Hyper K Banhatti Index for $G = HM_n$, $n \geq 3$ is given by $HB_1(HM_n) = 342n$ & $HB_2(HM_n) = 756n$.*

Proof:

Through the using of Table 3.1 for $HB_1(HM_n)$ and $HB_2(HM_n)$ and Table 4.3, we get

$$\begin{aligned}
HB_1(HM_n) &= \sum_{st\in G}(\alpha(s)+\alpha(t))^2 \\
&= 4n((2+3)+(3+3))^2+n((3+4)+(3+4))^2
\end{aligned}$$

We have,

$$\begin{aligned}
HB_1(HM_n) &= 324n. \\
HB_2(HM_n) &= \sum_{st\in G}(\alpha(s)\times\alpha(t))^2 \\
&= 4n((2\times 3)+(3\times 3))^2+n((3\times 4)+(3\times 4))^2
\end{aligned}$$

Hence,

$$HB_2(HM_n) = 756n.$$

Theorem 4.2.5. *The first and second Hyper K Banhatti Index for $G = HM_n$, $n \geq 3$ is given* *by $SB(HM_n) = 1.0427n$. Proof:*

With a Table 3.1 for $SB(HM_n)$ and Table 4.3, we reach

$$\begin{aligned} SB(HM_n) &= \sum_{st\in G} \frac{1}{(\alpha(s)+\alpha(t))^{\frac{1}{2}}} \\ &= 4n\left(\frac{1}{((2+3)+(3+3))^{\frac{1}{2}}}\right)+n\left(\frac{1}{((3+4)+(3+4)^{\frac{1}{2}})}\right) \\ SB(HM_n) &= 1.0427n. \end{aligned}$$

Hence, I figured out some degree based topological indices for my graph Mobius strip. Next, I'm going to graphical comparison of topological indices with their entropies in section 4.3.1 and with heat of formation in section 4.3.2.

Lemma 4.2.6. *Consider a connected graph called G with n vertices. For each vertex, n_i tells us how many edges are connected to it (which is its degree) and m_{ij} tells how many edges connecting with vertices with degrees i and j together [31].*

$$\overline{E}_{ij} = \{uv \in E(\overline{G}) | \ \widetilde{\phi}(v) = i, \ \widetilde{\phi}(u) = j\}$$

$$\overline{m}_{ij} = |\overline{E}_{ij}| = \begin{cases} \frac{n_i(n_i-1)}{2} - m_{ii}, & i = j \\ n_i n_j - m_{ij}, & i < j \end{cases}$$

Now, let's look at derivation of topological co indices for Hexagonal Mobius Strip. We'll use the information provided in Table 4.3 and the mentioned lemma.

For $i = 2$, $j = 3$: taking values of n_2, n_3 and m_{23} form 4.1 and 4.2.

$$\begin{aligned} \overline{m}_{23} &= n_2 n_3 - m_{23} \\ &= 2n \times 2n - 4n \\ \overline{m}_{23} &= 4n^2 - 4n \end{aligned}$$

For $i = 3,\ j = 3$: taking values of n_3, n_3 and m_{33} form 4.1 and 4.2.

$$\begin{aligned}
\overline{m}_{33} &= \frac{n_3(n_3-1)}{2} - m_{33} \\
&= \frac{2n(2n-1)}{2} - n \\
\overline{m}_{33} &= 2n^2 - 2n
\end{aligned}$$

Table 4.4: Edge-Partitioning of $\overline{HM_n}$

$Frequency$	$(\alpha(s), \alpha(t))$
$4n^2 - 4n$	$(2,3)$
$2n^2 - 2n$	$(3,3)$

Theorem 4.2.7. *The first and second Zagreb Co Index for $G = HM_n$, $n \geq 3$ is given by $\overline{M_1}(HM_n) = 32n^2 - 32n$ & $\overline{M_2}(HM_n) = 42n^2 - 42n$.*

Proof:

By use of Table 3.2 for $\overline{M_1}(HM_n)$ and $\overline{M_2}(HM_n)$ and Table 4.4, we access

$$\begin{aligned}
\overline{M_1}(HM_n) &= \sum_{st \in G} (\alpha(s) + \alpha(t)) \\
&= (4n^2 - 4n)(2+3) + (2n^2 - 2n)(3+3) \\
\overline{M_1}(HM_n) &= 32n^2 - 32n. \\
\overline{M_2}(HM_n) &= \sum_{st \in G} (\alpha(s) \times \alpha(t)) \\
&= (4n^2 - 4n)(2 \times 3) + (2n^2 - 2n)(3 \times 3) \\
\overline{M_2}(HM_n) &= 42n^2 - 42n.
\end{aligned}$$

Theorem 4.2.8. *The Hyper Zagreb Co Index for $G = HM_n$, $n \geq 3$ is given by $\overline{HM}(HM_n) = 172n^2 - 172n$.*

Proof:

Via using Table 3.2 for $\overline{HM}(HM_n)$ and Table 4.4, we obtain

$$\begin{aligned}
\overline{HM}(HM_n) &= \sum_{st\in G}(\alpha(s)+\alpha(t))^2 \\
&= (4n^2-4n)(2+3)^2+(2n^2-2n)(3+3)^2 \\
\overline{HM}(HM_n) &= 172n^2-172n.
\end{aligned}$$

Theorem 4.2.9. *The Forgotten Co Index for $G = HM_n$, $n \geq 3$ is given by $\overline{F}(HM_n) = 88n^2 - 88n$.*

Proof:

Table 3.2 for $\overline{F}(HM_n)$ and Table 4.4 helps us to get

$$\begin{aligned}
\overline{F}(HM_n) &= \sum_{st\in G}(\alpha(s)^2+\alpha(t)^2) \\
&= (4n^2-4n)(2^2+3^2)+(2n^2-2n)(3^2+3^2) \\
\overline{F}(HM_n) &= 88n^2-88n.
\end{aligned}$$

Theorem 4.2.10. *The first and second Multiple Zagreb Co Index for $G = HM_n$, $n \geq 3$ is given by $\overline{PM_1}(HM_n) = 240n^4 - 480n^3 + 240n^2$, $\overline{PM_2}(HM_n) = 432n^4 - 864n^3 + 432n^2$.*

Proof:

With the help of Table 3.2 for $\overline{PM_1}(HM_n)$ and $\overline{PM_2}(HM_n)$ and Table 4.4, we gain

$$\begin{aligned}
\overline{PM_1}(HM_n) &= \prod_{st\in G}(\alpha(s)+\alpha(t)) \\
&= (4n^2-4n)(2+3)\times(2n^2-2n)(3+3) \\
\overline{PM_1}(HM_n) &= 240n^4-480n^3+240n^2. \\
\overline{PM_2}(HM_n) &= \prod_{st\in G}(\alpha(s)\times\alpha(t)) \\
&= (4n^2-4n)(2\times 3)\times(2n^2-2n)(3\times 3) \\
\overline{PM_2}(HM_n) &= 432n^4-864n^3+432n^2.
\end{aligned}$$

Theorem 4.2.11. *The Randic Co Index for $G = HM_n$, $n \geq 3$ is given by*

$\overline{R_{\frac{-1}{2}}}(HM_n) = 2.2997n^2 - 2.2997n$, $\overline{R_{-1}}(HM_n) = 0.8889n^2 - 0.8889n$, $\overline{R_{\frac{1}{2}}}(HM_n) = 15.7980n^2 - 15.7980n$ & $\overline{R_1}(HM_n) = 42n^2 - 42n$.

Proof:

By consulting Table 3.2 for $\overline{R_{\frac{-1}{2}}}(HM_n)$, $\overline{R_{-1}}(HM_n)$, $\overline{R_{\frac{1}{2}}}(HM_n)$ and $\overline{R_1}(HM_n)$ and Table 4.4. The general form of Randic co index,

$$\overline{R_\beta}(HM_n) \quad = \quad \sum_{st \in HM_n} (\alpha(s) \times \alpha(t))^\beta, where \beta = (\frac{-1}{2}, -1, 1, \frac{1}{2})$$

$$\begin{aligned}
&\textit{If } \beta = \frac{-1}{2} \textit{then},\\
\overline{R_{\frac{-1}{2}}}(HM_n) &= \sum_{st \in G} (\alpha(s) \times \alpha(t))^{\frac{-1}{2}}\\
&= (4n^2 - 4n)(2 \times 3)^{\frac{-1}{2}} + (2n^2 - 2n)(3 \times 3)^{\frac{-1}{2}}\\
\overline{R_{\frac{-1}{2}}}(HM_n) &= 2.2997n^2 - 2.2997n.\\
&\textit{If } \beta = -1 \textit{then},\\
\overline{\overline{R_{-1}}}(HM_n) &= \sum_{st \in G} (\alpha(s) \times \alpha(t))^{-1}\\
&= (4n^2 - 4n)(2 \times 3)^{-1} + (2n^2 - 2n)(3 \times 3)^{-1}\\
\overline{R_{-1}}(HM_n) &= 0.8889n^2 - 0.8889n.\\
&\textit{If } \beta = \frac{1}{2} \textit{then},\\
\overline{R_{\frac{1}{2}}}(HM_n) &= \sum_{st \in G} (\alpha(s) \times \alpha(t))^{\frac{1}{2}}\\
&= (4n^2 - 4n)(2 \times 3)^{\frac{1}{2}} + (2n^2 - 2n)(3 \times 3)^{\frac{1}{2}}\\
\overline{R_{\frac{1}{2}}}(HM_n) &= 15.7980n^2 - 15.7980n.\\
&\textit{If } \beta = 1 \textit{ then},\\
\overline{\overline{R_1}}(HM_n) &= \sum_{st \in G} (\alpha(s) \times \alpha(t))^1\\
&= (4n^2 - 4n)(2 \times 3) + (2n^2 - 2n)(3 \times 3)\\
\overline{R_1}(HM_n) &= 42n^2 - 42n.
\end{aligned}$$

Here, I came up after calculating topological co indices for Mobius strip graph. Now, I’m planning to compare topological co indices with their entropies in section 4.3.3 and with heat of formation in section 4.3.4 in the form of graph by using curve fitting method. after all the calculations, I have included tables that show the results of our calculations for the corresponding topological indices and co indices in Table 4.5, 4.6, 4.7 and 4.8.

Here, I specify the determination of entropy values, which are derived from calculations

Table 4.5: Comparison of B_1, B_2, HB_1, HB_2 and SB indicators for HM_n

$[n]$	B_1	B_2	HB_1	HB_2	SB
3	174	252	1026	2268	3.1281
4	232	336	1368	3024	4.1708
5	290	420	1710	3780	5.2135
6	348	504	2052	4536	$6,2562$
7	406	588	2394	5292	7.2989
8	464	672	2736	6048	8.3416
9	522	756	3078	6804	9.3843
10	580	840	7560	7560	10.427

Table 4.6: Comparison of MB_1, MB_2, $ReZG_1$, $ReZG_2$ and $ReZG_3$ indicators for HM_n

$[n]$	MB_1	MB_2	$ReZG_1$	$ReZG_2$	$ReZG_3$
3	1.3052	0.9250	12	18.9	522
4	1.7403	1.2333	16	25.2	696
5	2.1753	1.5417	20	31.5	870
6	2.6104	1.8500	24	37.8	1044
7	3.0455	2.1583	28	44.1	1218
8	3.4805	2.4667	32	50.4	1392
9	3.9156	2.7750	36	56.7	1566
10	4.3506	3.0833	40	63	1740

Table 4.7: Comparison of $\overline{M_1}$, $\overline{M_2}$, $\overline{HM}$, $\overline{PM_1}$ and $\overline{PM_2}$ indicators for $\overline{HM_n}$

$[n]$	$\overline{M_1}$	$\overline{M_2}$	$\overline{HM}$	$\overline{PM_1}$	$\overline{PM_2}$
3	192	252	1032	8640	15552
4	384	504	2064	34560	62208
5	640	840	3440	96000	172800
6	960	1260	5160	216000	388800
7	1344	1764	7224	423360	762048
8	1792	2352	9632	752640	1354752
9	2304	3024	12384	1244160	2239488
10	2880	3780	15480	1944000	3499200

Table 4.8: Comparison of $\overline{F}$, $\overline{R_{\frac{-1}{2}}}$, $\overline{R_{-1}}$, $\overline{R_{\frac{1}{2}}}$ and $\overline{R_1}$ indicators for $\overline{HM_n}$

$[n]$	$\overline{F}$	$\overline{R_{\frac{-1}{2}}}$	$\overline{R_{-1}}$	$\overline{R_{\frac{1}{2}}}$	$\overline{R_1}$
3	528	13.7982	5.3333	94.788	252
4	1056	27.5964	10.6667	189.576	504
5	1760	45.9940	17.7778	315.96	840
6	2640	68.9910	26.6667	473.94	1260
7	3696	96.5874	37.3333	663.516	1764
8	4928	128.7832	49.7778	884.688	2352
9	6336	165.5784	64	1137.456	3024
10	7920	206.9730	80	1421.82	3780

involving their corresponding topological indices.

$$
\begin{aligned}
E_{ReZG_1}(HM_n) &= log(4n)-\frac{1}{4n}[(5/6)(4n)log(5/6)+(6/9)(n)log(6/9)] \\
E_{ReZG_2}(HM_n) &= log\left(\frac{63n}{10}\right)-\frac{1}{\frac{63n}{10}}[(6/5)(4n)log(6/5)+(9/6)(n)log(9/6)] \\
E_{ReZG_3}(HM_n) &= log(174n)-\frac{1}{174n}[(30)(4n)log(30)+(54)(n)log(54)] \\
E_{B_1}(HM_n) &= log(58n)-\frac{1}{58n}\times[(11)(4n)log(11)+(14)(n)log(14)] \\
E_{B_2}(HM_n) &= log(84n)-\frac{1}{84n}[(15)(4n)log(15)+(24)(n)log(24)] \\
E_{MB_1}(HM_n) &= log\left(\frac{67}{154}n\right)-\frac{1}{\frac{67}{154}n}\times[(\frac{1}{11})(4n)log(\frac{1}{11})+(\frac{1}{14})(n)log(\frac{1}{14}) \\
E_{MB_2}(HM_n) &= log\left(\frac{37}{120}n\right)-\frac{1}{\frac{37}{120}n}\times[(\frac{1}{15})(4n)log(\frac{1}{15})+(\frac{1}{24})(n)log(\frac{1}{24}) \\
E_{HB_1}(HM_n) &= log(342n)-\frac{1}{342n}\times[(61)(4n)log(61)+(98)(n)log(98) \\
E_{HB_2}(HM_n) &= log(756n)-\frac{1}{756n}\times[(117)(4n)log(117)+(288)(n)log(288) \\
E_{SB}(HM_n) &= log(1.0427n)-\frac{1}{1.0427n}[(0.2134)(4n)log(0.2134) \\
&+ (0.1890)(n)log(0.1890)]
\end{aligned}
$$

Now, I figuring out entropy values, these values come from doing calculations related to

Table 4.9: Comparison of E_{B_1}, E_{B_2}, E_{HB_1}, E_{HB_2} and SB for HM_n

$[n]$	E_{B_1}	E_{B_2}	E_{HB_1}	E_{HB_2}	E_{SB}
3	1.1739	1.1670	1.1668	1.1384	1.1756
4	1.2988	1.2919	1.2918	1.2634	1.3005
5	1.3957	1.3888	1.3887	1.3603	1.3974
6	1.4749	1.4680	1.4678	1.4395	1.4766
7	1.5419	1.5350	1.5348	1.5064	1.5436
8	1.5998	1.5930	1.5928	1.5644	1.6015
9	1.6510	1.6441	1.6439	1.6155	1.6527
10	1.6968	1.6899	1.6897	1.6613	1.6985

Table 4.10: Comparison of E_{MB_1}, E_{MB_2}, E_{ReZG_1}, E_{ReZG_2} and E_{ReZG_3} for HM_n

$[n]$	E_{MB_1}	E_{MB_2}	E_{ReZG_1}	E_{ReZG_2}	E_{ReZG_3}
3	1.1743	1.1698	1.1745	1.1742	1.1613
4	1.2992	1.2948	1.2995	1.2991	1.2863
5	1.3961	1.3917	1.3964	1.3961	1.3832
6	1.4753	1.4708	1.4755	1.4752	1.4624
7	1.5422	1.5378	1.5425	1.5422	1.5293
8	1.6002	1.5958	1.6005	1.6002	1.5873
9	1.6514	1.6469	1.6516	1.6513	1.6384
10	1.6971	1.6927	1.6974	1.6971	1.6842

their respective topological co indices.

$$\begin{aligned}
E_{\overline{M_1}}(HM_n) &= log(32n^2-32n)-\frac{1}{32n^2-32n} \\
&\times [(5)(4n^2-4n)log(5)+(6)(2n^2-2n)log(6)] \\
E_{\overline{M_2}}(HM_n) &= log(42n^2-42n)-\frac{1}{42n^2-42n} \\
&\times [(6)(4n^2-4n)log(6)+(9)(2n^2-2n)log(9)] \\
E_{\overline{HM}}(HM_n) &= log(172n^2-172n)-\frac{1}{172n^2-172n} \\
&\times [(25)(4n^2-4n)log(25)+(36)(2n^2-2n)log(36)] \\
E_{\overline{PM_1}}(HM_n) &= log(240n^4-480n^3+240n^2)-\frac{1}{240n^4-480n^3+240n^2} \\
&\times [(5)(4n^2-4n)log(5)+(6)(2n^2-2n)log(6)] \\
E_{\overline{PM_2}}(HM_n) &= log(432n^4-864n^3+432n^2)-\frac{1}{432n^4-864n^3+432n^2} \\
&\times [(6)(4n^2-4n)log(6)+(9)(2n^2-2n)log(9)]
\end{aligned}$$

$$
\begin{aligned}
E_{\overline{F}}(HM_n) &= log(88n^2-88n)-\frac{1}{88n^2-88n} \\
&\times \;[(13)(4n^2-4n)log(13)+(18)(2n^2-2n)log(18)] \\
E_{\overline{R_{\frac{-1}{2}}}}(HM_n) &= log(2.2997n^2-2.2997n)-\frac{1}{2.2997n^2-2.2997n} \\
&\times \;\left[\frac{1}{6^{\frac{1}{2}}}(4n^2-4n)log\left(\frac{1}{6^{\frac{1}{2}}}\right)+\frac{1}{9^{\frac{1}{2}}}(2n^2-2n)log\left(\frac{1}{9^{\frac{1}{2}}}\right)\right] \\
E_{\overline{R_{-1}}}(HM_n) &= log\left(\frac{8}{9}n^2-\frac{8}{9}n\right)-\frac{1}{\frac{8}{9}n^2-\frac{8}{9}n} \\
&\times \;\left[\frac{1}{6}(4n^2-4n)log\left(\frac{1}{6}\right)+\frac{1}{9}(2n^2-2n)log\left(\frac{1}{9}\right)\right] \\
E_{\overline{R_{\frac{1}{2}}}}(HM_n) &= log(15.7980n^2-15.7980n)-\frac{1}{15.7980n^2-15.7980n} \\
&\times \;\left[(6)^{\frac{1}{2}}(4n^2-4n)log((6)^{\frac{1}{2}})+(9)^{\frac{1}{2}}(2n^2-2n)log((9)^{\frac{1}{2}})\right] \\
E_{\overline{R_1}}(HM_n) &= log(42n^2-42n)-\frac{1}{42n^2-42n} \\
&\times \;[6(4n^2-4n)log(6)+9(2n^2-2n)log(9)]
\end{aligned}
$$

The amount of heat absorbed or evolved when one mole of a compound is formed from its

Table 4.11: Comparison of $E_{\overline{M_1}}$, $E_{\overline{M_2}}$, $E_{\overline{HM}}$, $E_{\overline{PM_1}}$ and $E_{\overline{PM_2}}$ for $\overline{HM_n}$

$[n]$	$E_{\overline{M_1}}$	$E_{\overline{M_2}}$	$E_{\overline{HM}}$	$E_{\overline{PM_1}}$	$E_{\overline{PM_2}}$
3	1.5546	1.5478	1.5494	3.9203	4.1780
4	1.8557	1.8488	1.8505	4.5305	4.7869
5	2.0775	2.0707	2.0723	4.9774	5.2334
6	2.2536	2.2468	2.2484	5.3312	5.5870
7	2.3997	2.3929	2.3945	5.6244	5.8800
8	2.5247	2.5178	2.5195	5.8749	6.1304
9	2.6338	2.6270	2.6286	6.0935	6.3490
10	2.7307	2.7239	2.7255	6.2876	6.5430

constituent elements. And the standard ebthalpy of formation measured in units of energy per amount of substance, usually calculated in kJ/mol. We used Avogagro's number to figure out the enthalpy (a measure of energy) for one unit of a Hexagonal Mobius strip, and we found it to be $49.04kJ/mol$. Then, to get the total energy for the entire cell, we multiplied this value by the number of formula units in the cell. Additionally, we noticed that the heat of formation (a measure of the stability of a chemical compound) for the

Table 4.12: Comparison of $E_{\overline{F}}$, $E_{\overline{R_{\frac{-1}{2}}}}$,$E_{\overline{R_{-1}}}$, $E_{\overline{R_{\frac{1}{2}}}}$ and $E_{\overline{R_1}}$ for $\overline{HM_n}$

$[n]$	$E_{\overline{F}}$	$E_{\overline{R_{\frac{-1}{2}}}}$	$E_{\overline{R_{-1}}}$	$E_{\overline{R_{\frac{1}{2}}}}$	$E_{\overline{R_1}}$
3	1.5509	1.6481	1.5492	2.0263	1.5478
4	1.8519	1.9115	1.8502	2.2099	1.8488
5	2.0738	2.1152	2.0721	2.3619	2.0707
6	2.2498	2.2811	2.2481	2.4913	2.2468
7	2.3960	2.4208	2.3943	2.6041	2.3929
8	2.5209	2.5415	2.5192	2.7039	2.5178
9	2.6301	2.6476	2.6284	2.7934	2.6270
10	2.7270	2.7423	2.7253	2.8746	2.7239

Hexagonal Mobius strip as we increase the number of cells. Specially, as the number of formula units goes from [3] to [10],the heat of formation decreases from 0.7329×10^{-21} to 8.1435×10^{-21}.

Table 4.13: Heat of Formation of $\overline{HM_n}$

$[n]$	$Units$	HoF
[3]	9	0.7329×10^{-21}
[4]	16	1.3030×10^{-21}
[5]	25	2.0359×10^{-21}
[6]	36	2.9317×10^{-21}
[7]	49	3.9903×10^{-21}
[8]	64	5.2118×10^{-21}
[9]	81	6.5962×10^{-21}
[10]	100	8.1435×10^{-21}

4.3 Rational Curve Fitting Between Indices/Co Indices and Entropy

We are using a special method called rational curve fitting to see how entropy/HoF (Heat of Formation) is connected to different system indicators. Curve fitting can be used as an aid for data visualization, to infer values of a function where no data are available, and to summarize the relationship among two or more variables.To do this, we made a special math model using rational curve fitting that helps us find patterns and connections between entropy/HoF and these indicators more easily. Specifically, we are studying how entropy/Hof relates to indicators named Redefined Zagreb & K Banhatti indices and Randic, Forgotten and Zagreb co indices. In this process, we are looking at three important things: root mean squared error (RMSE), R^2 and sum of squared error (SSE). Lower values mean our results are more accurate, and if the R^2 value is closed to 1, it shows thar our line fits the data points well.

We are mainly interested in how closely connected Redefined Zagreb & K Banhatti indices and Randic, Forgotten and Zagreb co indices are their respective entropies/HoF for HM_n. we have put the results in tables 4.14, 4.15, 4.16 and 4.17 respectively, making it easier for us to see how strongly these variables are linked based on the measures we talked about

Table 4.14: Connection Between Indices and Entropies for HM_n

$Indicators$	$FitType$	SSE	R^2	$Adjusted-R^2$	$RMSE$
B_1	$Rat24$	1.487×10^{-7}	1	1	0.0003857
B_2	$Rat32$	2.85×10^{-7}	1	1	0.0003775
HB_1	$Rat24$	3.997×10^{-8}	1	1	0.0001999
HB_2	$Rat24$	4.839×10^{-8}	1	1	0.00022
SB	$Rat23$	1.974×10^{-5}	0.9999	0.9997	0.003141
MB_1	$Rat14$	3.459×10^{-7}	1	1	0.0004159
MB_2	$Rat24$	8.354×10^{-7}	1	1	0.000914
$ReZG_1$	$Rat24$	1.22×10^{-7}	1	1	0.0003493
$ReZG_2$	$Rat33$	1.617×10^{-8}	1	1	0.0001272
$ReZG_3$	$Rat24$	4.297×10^{-7}	1	1	0.0006555

Table 4.15: Connection between indicators and HoF for HM_n

$Indicators$	$FitType$	SSE	R^2	$RMSE$
B_1	$Rat22$	3.158×10^{-7}	1	0.0003245
B_2	$Rat24$	3.64×10^{-5}	1	0.006033
HB_1	$Rat23$	1.31×10^{-6}	1	0.0008094
HB_2	$Rat31$	5.446×10^{-9}	1	0.00004261
SB	$Rat23$	5.228×10^{-4}	1	0.01617
MB_1	$Rat23$	5.572×10^{-4}	1	0.01669
MB_2	$Rat22$	1.023×10^{-6}	1	0.000584
$ReZG_1$	$Rat23$	5.231×10^{-4}	1	0.01617
$ReZG_2$	$Rat23$	8.953×10^{-5}	1	0.006691
$ReZG_3$	$Rat15$	1.531×10^{-8}	1	0.0001237

4.3.1 Models of Indices and Entropies by Using Rational Curve Fitting

We are discussing how we use a method called rational curve fitting to create models for different indices and entropies. This helps us understand and represent the relationships

Table 4.16: Connection between co indices and entropies for $\overline{HM_n}$

$Indicators$	$FitType$	SSE	R^2	$Adjusted-R^2$	$RMSE$
$\overline{M_1}$	$Rat32$	4.475×10^{-8}	1	1	0.0001496
$\overline{M_2}$	$Rat22$	7.449×10^{-7}	1	1	0.0004983
$\overline{HM}$	$Rat33$	1.525×10^{-8}	1	1	0.0001235
$\overline{PM_1}$	$Rat33$	2.985×10^{-7}	1	1	0.0005463
$\overline{PM_2}$	$Rat33$	2.864×10^{-7}	1	1	0.0005352
$\overline{F}$	$Rat24$	5.833×10^{-6}	1	1	0.002415
$\overline{R_{\frac{-1}{2}}}$	$Rat22$	5.783×10^{-7}	1	1	0.0004391
$\overline{R_{-1}}$	$Rat22$	7.111×10^{-7}	1	1	0.0004869
$\overline{R_{\frac{1}{2}}}$	$Rat32$	1.399×10^{-9}	1	1	2.645×10^{-5}
$\overline{R_1}$	$Rat32$	1.972×10^{-8}	1	1	9.93×10^{-5}

Table 4.17: Connection between co indices and HoF for $\overline{HM_n}$

$Indicators$	$FitType$	SSE	R^2	$RMSE$
$\overline{M_1}$	$Rat22$	2.55×10^{-7}	1	0.0002916
$\overline{M_2}$	$Rat22$	2.379×10^{-7}	1	0.0002816
$\overline{HM}$	$Rat24$	7.413×10^{-8}	1	0.0002723
$\overline{PM_1}$	$Rat32$	1.114×10^{-4}	1	0.007464
$\overline{PM_2}$	$Rat32$	1.114×10^{-4}	1	0.007464
$\overline{R_{\frac{-1}{2}}}$	$Rat32$	3.418×10^{-9}	1	4.134×10^{-5}
$\overline{R_{-1}}$	$Rat32$	6.776×10^{-8}	1	0.0001841
$\overline{R_{\frac{1}{2}}}$	$Rat22$	4.705×10^{-7}	1	0.000396
$\overline{R_1}$	$Rat15$	1.574×10^{-7}	1	0.0003967
$\overline{F}$	$Rat24$	6.131×10^{-7}	1	0.000783

between these factors in a simple way.

$$E(B_1)=\frac{p_1(B_1)^2+p_2(B_1)+p_3}{(B_1)^4+q_1(B_1)^3+q_2(B_1)^2+q_3(B_1)+q_4}$$

Where $p_1=601.2$, $CB=(-5514,6717)$. $p_2=1294$, $CB=(-1.149e+04,1.408e+04)$. $p_3=-979.7$, $CB=(-1.706e+04,1.51e+04)$. $q_1=-8.717$, $CB=(-69.53,52.09)$. $q_2=284.4$, $CB=(-2559,3127)$. $q_3=927.8$, $CB=(-8483,1.034e+04)$ and $q_4=-649$, $CB=(-1.13e+04,1e+04)$.

$$E(B_2)=\frac{p_1(B_2)^3+p_2(B_2)^2+p_3(B_2)+p_4}{(B_2)^2+q_1(B_2)+q_2}$$

Where $p_1 = 0.0515$, $CB = (-3.494, 3.597)$. $p_2 = 2.572$, $CB = (-235.2, 240.4)$. $p_3 = 28.16$, $CB = (-1.182e+04, 1.188e+04)$. $p_4 = 60.88$, $CB = (-3.206e+04, 3.218e+04)$. $q_1 = 14.33$, $CB = (-5551, 5580)$ and $q_2 = 40.51$, $CB = (-2.133e+04, 2.141e+04)$.

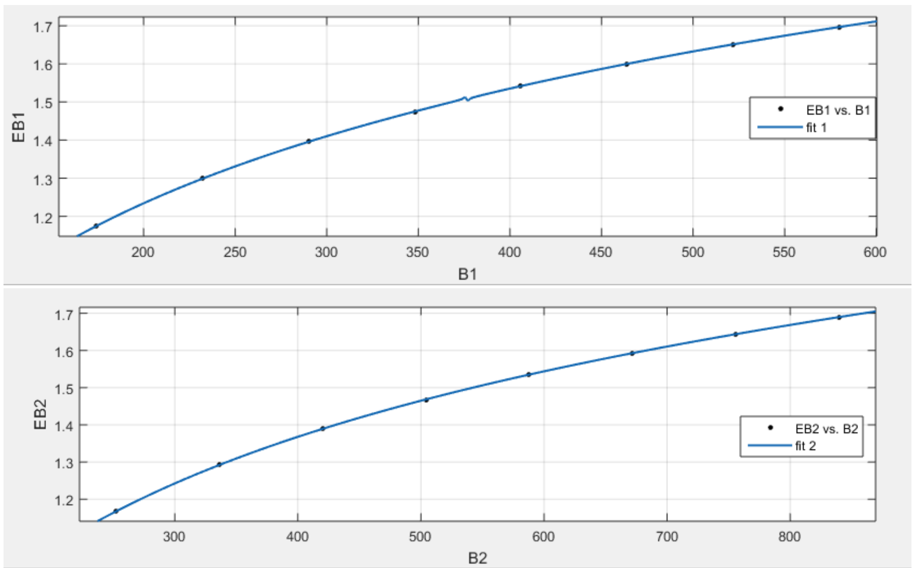


Figure 4.1: (B_1) vs (E_{B_1}) and (B_2) vs (E_{B_2}) for HM_n

$$E(HB_1) = \frac{p_1(HB_1)^2 + p_2(HB_1) + p3}{(HB_1)^4 + q_1(HB_1)^3 + q_2(HB_1)^2 + q_3(HB_1) + q_4}$$

Where $p_1 = 567.7$, $CB = (-2287, 3422)$. $p_2 = 1350$, $CB = (-1.646e+04, 1.916e+04)$. $p_3 = -539.4$, $CB = (-3.465e+04, 3.357e+04)$. $q_1 = -8.383$, $CB = (-33.09, 16.33)$. $q_2 = 268.4$, $CB = (-965.8, 1503)$. $q_3 = 937.7$, $CB = (-8711, 1.059e+04)$. and $q_4 = -359$, $CB = (-2.306e+04, 2.234e+04)$.

$$E(HB_2) = \frac{p_1(HB_2)^2 + p_2(HB_2) + p_3}{(HB_2)^4 + q_1(HB_2)^3 + q_2(HB_2)^2 + q_3(HB_2) + q_4}$$

Where $p_1 = 565.2$, $CB = (-3105, 4235)$. $p_2 = 1758$, $CB = (-1.808e+04, 2.16e+04)$. $p_3 = 607.9$, CB=$(-2.837e+04, 2.959e+04)$. $q_1 = -7.79$, $CB = (-36.34, 20.76)$. $q_2 = 264.7$, $CB = (-1332, 1861)$. $q_3 = 1147$, $CB = (-1.027e+04, 1.256e+04)$. and $q_4 = 412.4$, $CB = (-1.924e+04, 2.007e+04)$.

$$E(SB) = \frac{p_1(SB)^2 + p_2(SB) + p_3}{(SB)^3 + q_1(SB)^2 + q_2(SB) + q_3}$$

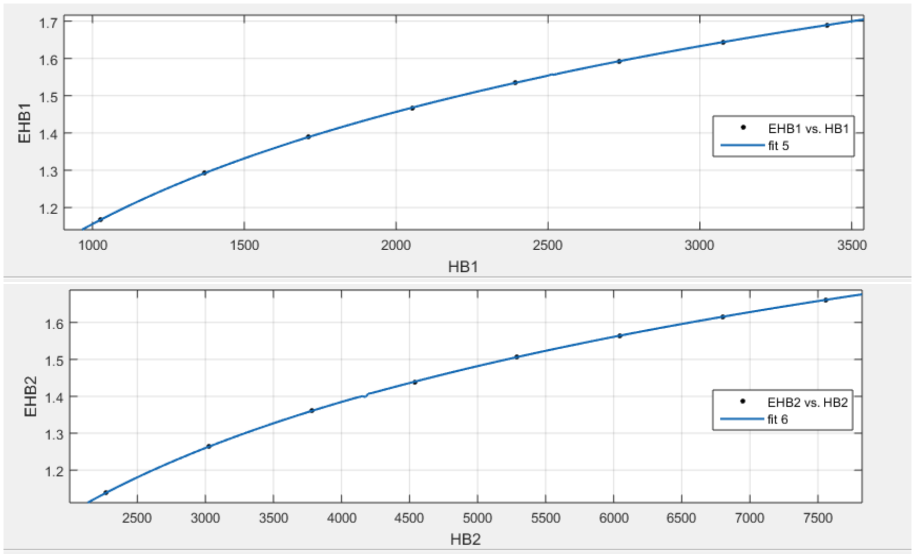


Figure 4.2: (HB_1) vs (E_{HB_1}) and (HB_2) vs (E_{HB_2}) for HM_n

Where $p_1 = 2543$, $CB = (-2.542e+05, 2.593e+05)$. $p_2 = 9146$, $CB = (-9.103e+05, 9.286e+05)$, $p_3 = 3564$, $CB = (-3.524e+05, 3.596e+05)$. $q_1 = 1100$, $CB = (-1.102e+05, 1.124e+05)$. $q_2 = 5786$, $CB = (-5.761e+05, 5.877e+05)$. and $q_3 = 2356$, $CB = (-2.33e+05, 2.377e+05)$.

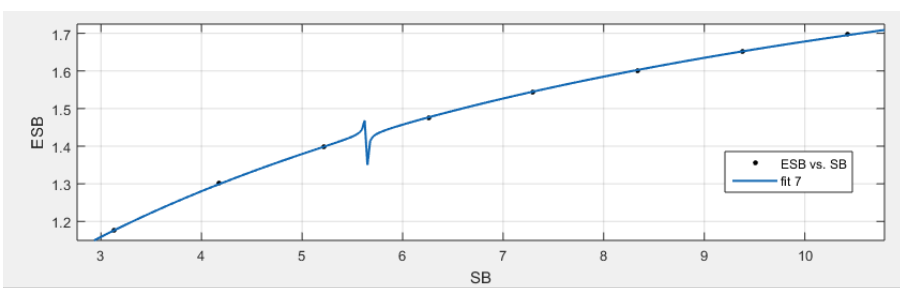


Figure 4.3: (SB) vs (E_{SB}) for HM_n

$$E(MB_1) = \frac{p_1(MB_1) + p_2}{(MB_1)^4 + q_1(MB_1)^3 + q_2(MB_1)^2 + q_3(MB_1) + q_4}$$

Where $p_1 = 363.9$, $CB = (-1261, 1988)$. $p_2 = 1255$, $CB = (-3305, 5815)$. $q_1 = -2.228$, $CB = (-4.85, 0.3942)$. $q_2 = 0.2755$, $CB = (-20.01, 20.56)$. $q_3 = 151.5$, $CB = (-598.2, 901.1)$. and $q_4 = 831.4$, $CB = (-2189, 3851)$.

$$E(MB_2) = \frac{p_1(MB_2)^2 + p_2(MB_2) + p_3}{(MB_2)^4 + q_1(MB_2)^3 + q_2(MB_2)^2 + q_3(MB_2) + q_4}$$

Where $p_1 = 63.66$, $CB = (-2.16e+04, 2.173e+04)$. $p_2 = 553.5$, $CB = (-6.386e+04, 6.497e+04)$. $p_3 = 1291$, $CB = (-3.147e+04, 3.405e+04)$. $q_1 = -3.167$, $CB = (-210.1, 203.7)$. $q_2 = 29.95$, $CB = (-9858, 9918)$. $q_3 = 275.2$, $CB = (-4.192e+04, 4.248e+04)$. and $q_4 = 857.3$, $CB = (-2.09e+04, 2.261e+04)$.

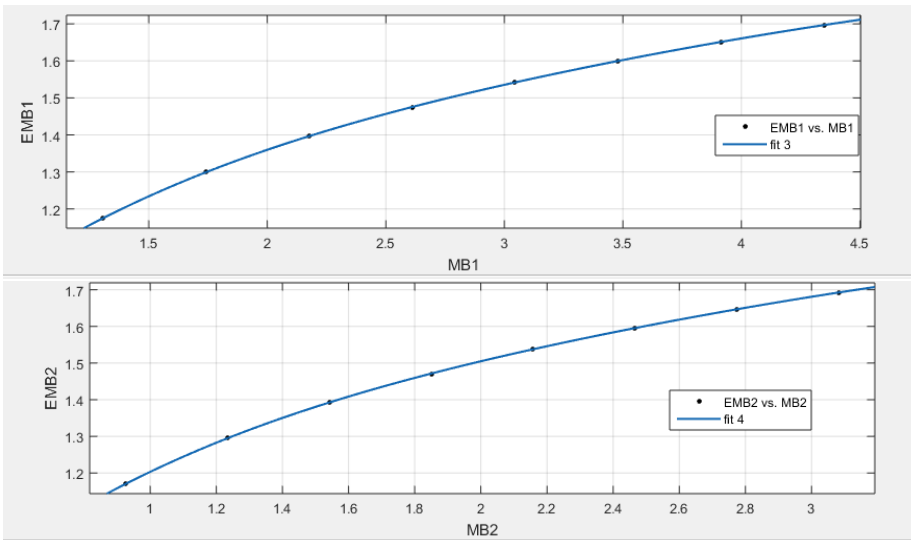


Figure 4.4: (MB_1) vs (E_{MB_1}) and (MB_2) vs (E_{MB_2}) for HM_n

$$E(ReZG_1) = \frac{p_1(ReZG_1)^2 + p_2(ReZG_1) + p_3}{(ReZG_1)^4 + q_1(ReZG_1)^3 + q_2(ReZG_1)^2 + q_3(ReZG_1) + q_4}$$

Where $p_1 = 624.4$, $CB = (-4925, 6174)$. $p_2 = 1356$, $CB = (-1.439e+04, 1.71e+04)$. $p_3 = -937.5$, $CB = (-1.622e+04, 1.434e+04)$. $q_1 = -9.455$, $CB = (-66.24, 47.33)$. $q_2 = 296.6$, $CB = (-2254, 2847)$. $q_3 = 965$, $CB = (-9364, 1.129e+04)$. and $q_4 = -620.8$, $CB = (-1.074e+04, 9496)$.

$$E(ReZG_2) = \frac{p_1(ReZG_2)^3 + p_2(ReZG_2)^2 + p_3(ReZG_2) + p_4}{(ReZG_2)^3 + q_1(ReZG_2)^2 + q_2(ReZG_2) + q_3}$$

Where $p_1 = 2.834$, $CB = (-0.267, 5.936)$. $p_2 = 29.93$, $CB = (-128.5, 188.3)$. $p_3 = 50.87$, $CB = (-578.4, 680.2)$, $p_4 = -26.12$, $CB = (-825.4, 773.2)$. $q_1 = 15.62$, $CB = (-56.91, 88.14)$. $q_2 = 35.56$, $CB = (-335.6, 406.8)$. and $q_3 = -17.3$, $CB = (-546.6, 512)$.

$$E(ReZG_3) = \frac{p_1(ReZG_3)^2 + p_2(ReZG_3) + p_3}{(ReZG_3)^4 + q_1(ReZG_3)^3 + q_2(ReZG_3)^2 + q_3(ReZG_3) + q_4}$$

Where $p_1 = 86.8, CB = (-1.452e+04, 1.47e+04)$. $p_2 = 629.1, CB = (-2.77e+04, 2.896e+04)$. $p_3 = 1235$, $CB = (-4.615e+04, 4.862e+04)$. $q_1 = -2.401$, $CB = (-174.5, 169.7)$. $q_2 = 38.12$, $CB = (-6901, 6978)$. $q_3 = 330.4$, $CB = (-2.098e+04, 2.164e+04)$. and $q_4 = 824.8$, $CB = (-3.083e+04, 3.248e+04)$.

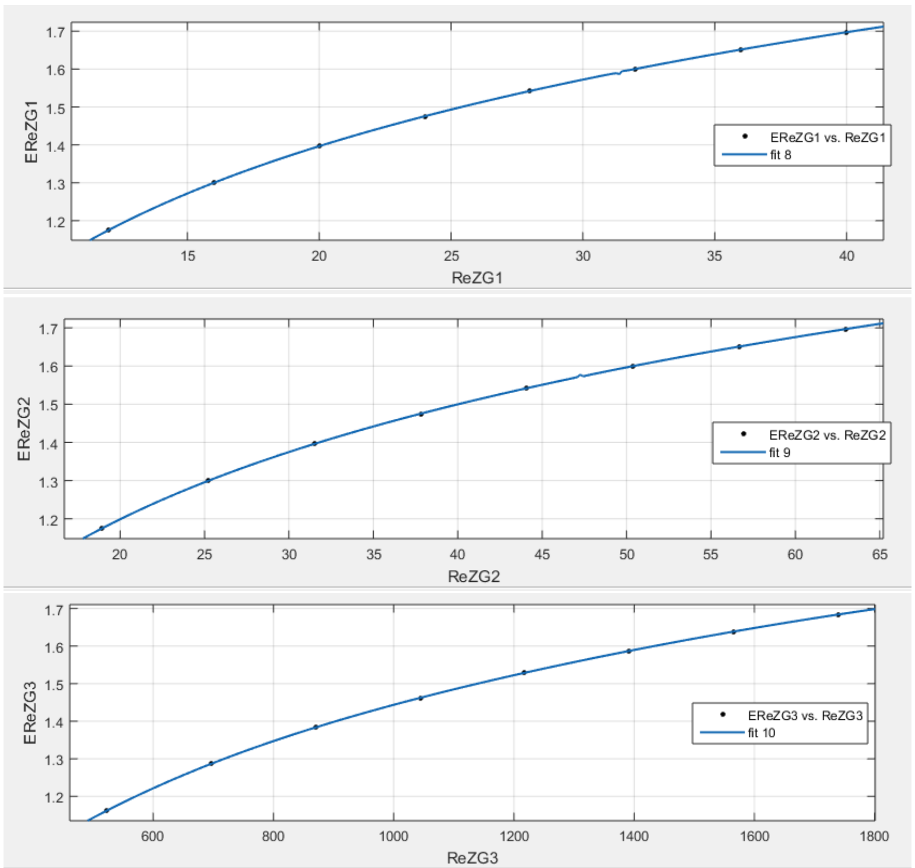


Figure 4.5: (ReZ_1) vs (E_{ReZ_1}), (ReZ_2) vs (E_{ReZ_2}) and (ReZ_3) vs (E_{ReZ_3}) for HM_n

4.3.2 Models Of Indices And Heat Of Formation By Using Curve Fitting:

$$HoF(B_1) = \frac{p_1(B_1)^2 + p_2(B_1) + p_3}{(B_1)^2 + q_1(B_1) + q_2}$$

Where $p_1 = 1863, CB = (-1.09e+04, 1.463e+04)$. $p_2 = 9899, CB = (-5.773e+04, 7.753e+04)$. $p_3 = 1.315e+04, CB = (-7.651e+04, 1.028e+05)$. $q_1 = -3.609, CB = (-16.17, 8.953)$.

and $q_2 = 3822$, $CB = (-2.224e+04, 2.988e+04)$.

$$HoF(B_2) = \frac{p_1(B_2)^2 + p_2(B_2) + p_3}{(B_2)^4 + q_1(B_2)^3 + q_2(B_2)^2 + q_3(B_3) + q_4}$$

Where $p_1 = -70.2$, $CB = (-1213, 1073)$. $p_2 = -58.71$, $CB = (-5502, 5384)$. $p_3 = 220.9$, $CB = (-6812, 7254)$. $q_1 = -5.789$, $CB = (-18.46, 6.882)$. $q_2 = 20.35$, $CB = (-55.98, 96.69)$. $q_3 = -65.65$, $CB = (-357.9, 226.6)$. and $q_4 = 64.19$, $CB = (-1980, 2108)$.

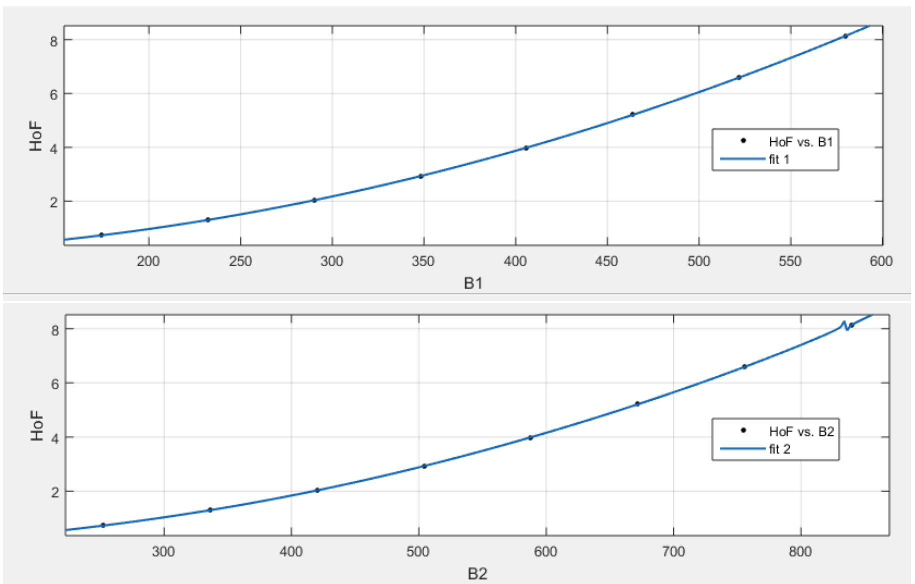


Figure 4.6: (B_1) vs HoF and (B_2) vs HoF for HM_n

$$HoF(HB_1) = \frac{p_1(HB_1)^2 + p_2(HB_1) + p_3}{(HB_1)^3 + q_1(HB_2)^2 + q_2(HB_2) + q_3}$$

Where $p_1 = 448.3$, $CB = (-3120, 4017)$. $p_2 = 2330$, $CB = (-1.699e+04, 2.165e+04)$. $p_3 = 3040$, $CB = (-2.288e+04, 2.896e+04)$. $q_1 = -4.131$, $CB = (-15.55, 7.289)$. $q_2 = 11.42$, $CB = (-55.7, 78.55)$. and $q_3 = 883.7$, $CB = (-6650, 8418)$.

$$HoF(HB_2) = \frac{p_1(HB_2)^3 + p_2(HB_2)^2 + p_3(HB_2) + p_4}{(HB_2) + q_1}$$

Where $p_1 = 0.4886$, $CB = (0.4885, 0.4887)$. $p_2 = 2.719$, $CB = (2.133, 3.305)$. $p_3 = 4.109$, $CB = (0.9994, 7.218)$. $p_4 = 0.8865$, $CB = (-3.239, 5.012)$. and $q_1 = 0.2577$, $CB = (-0.9414, 1.457)$.

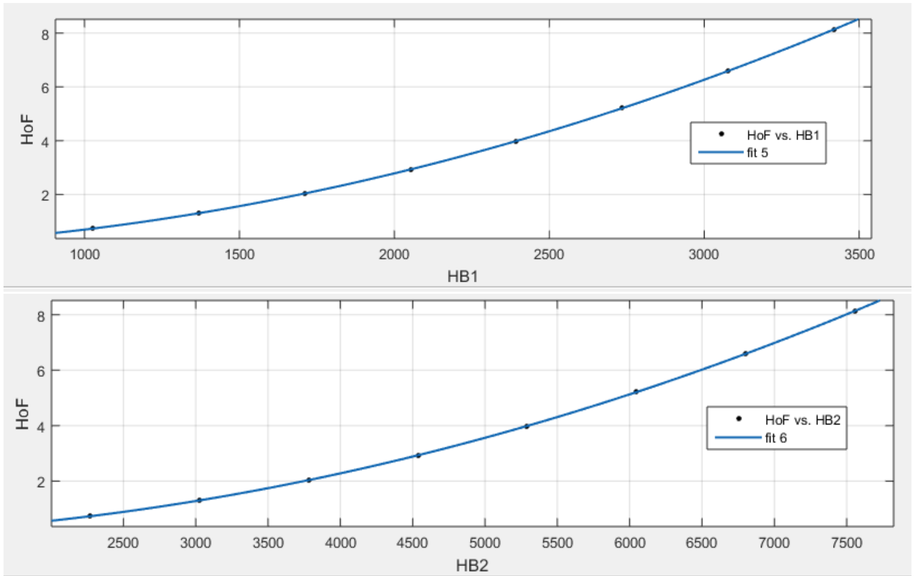


Figure 4.7: (HB_1) vs HoF and (HB_2) vs HoF for HM_n

$$HoF(SB) = \frac{p_1(SB)^2 + p_2(SB) + p_3}{(SB)^3 + q_1(SB)^2 + q_2(SB) + q_3}$$

Where $p_1 = 35.36$, $CB = (5.353, 65.38)$. $p_2 = 89.55$, $CB = (-37.49, 216.6)$, $p_3 = 33.34$, $CB = (-124.6, 191.3)$. $q_1 = -5.314$, $CB = (-7.258, -3.37)$. $q_2 = 18.83$, $CB = (8.813, 28.86)$. and $q_3 = 9.707$, $CB = (-36.2, 55.61)$.

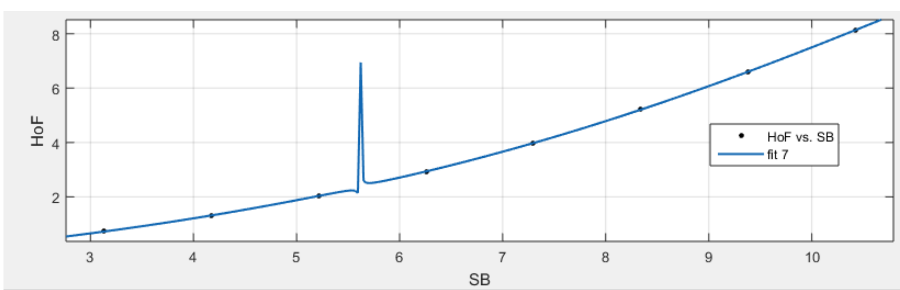


Figure 4.8: (SB) vs HoF for HM_n

$$HoF(MB_1) = \frac{p_1(MB_1)^2 + p_2(MB_1) + p_3}{(MB_1)^3 + q_1(MB_1)^2 + q_2(MB_1) + q_3}$$

Where $p_1 = 34.29$, $CB = (5.726, 62.86)$. $p_2 = 63.51$, $CB = (-49.4, 176.4)$. $p_3 = -16.42$, $CB = (-160.7, 127.9)$. $q_1 = -5.894$, $CB = (-7.789, -3.999)$. $q_2 = 22.14$, $CB = (10.93, 33.35)$. and $q_3 = -4.791$, $CB = (-46.73, 37.15)$.

$$HoF(MB_2) = \frac{p_1(MB_2)^2 + p_2(MB_2) + p_3}{(MB_2)^2 + q_1(MB_2) + q_2}$$

Where $p_1 = 1005$, $CB = (-5714, 7723)$. $p_2 = 5346$, $CB = (-3.019e+04, 4.088e+04)$. $p_3 = 7108$, $CB = (-3.998e+04, 5.42e+04)$. $q_1 = -3.677$, $CB = (-15.47, 8.112)$. and $q_2 = 2066$, $CB = (-1.162e+04, 1.575e+04)$.

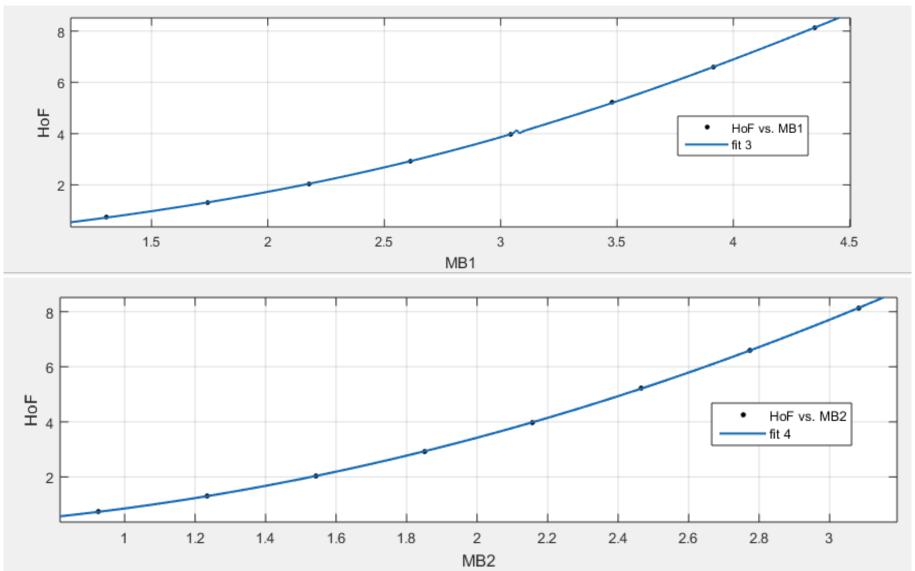


Figure 4.9: (MB_1) vs HoF and (MB_2) vs HoF for HM_n

$$HoF(ReZG_1) = \frac{p_1(ReZG_1)^2 + p_2(ReZG_1) + p_3}{(ReZG_1)^3 + q_1(ReZG_1)^2 + q_2(ReZG_1) + q_3}$$

Where $p_1 = 35.27$, $CB = (5.385, 65.15)$. $p_2 = 89.07$, $CB = (-37.47, 215.6)$. $p_3 = 32.72$, $CB = (-124.6, 190.1)$. $q_1 = -5.313$, $CB = (-7.245, -3.382)$. $q_2 = 18.83$, $CB = (8.856, 28.81)$. and $q_3 = 9.526$, $CB = (-36.2, 55.25)$.

$$HoF(ReZG_2) = \frac{p_1(ReZG_2)^2 + p_2(ReZG_2) + p_3}{(ReZG_2)^3 + q_1(ReZG_2)^2 + q_2(ReZG_2) + q_3}$$

Where $p_1 = 5890$, $CB = (-3.402e+06, 3.414e+06)$. $p_2 = 2.727e+04$, $CB = (-1.579e+07, 1.585e+07)$. $p_3 = 3.299e+04$, $CB = (-1.915e+07, 1.921e+07)$. $q_1 = -146.9$, $CB = (-8.255e+04, 8.225e+04)$. $q_2 = 721.3$, $CB = (-4.083e+05, 4.097e+05)$. and

$q_3 = 9576$, $CB = (-5.558e+06, 5.577e+06)$.

$$HoF(ReZG_3) = \frac{p_1(ReZG_3) + p_2}{(ReZG_3)^5 + q_1(ReZG_3)^4 + q_2(ReZG_3)^3 + q_3(ReZG_3)^2 + q_4(ReZG_3) + q_5}$$

Where $p_1 = -845.1$, $CB = (-2249, 558.4)$. $p_2 = -1969$, $CB = (-5159, 1222)$. $q_1 = -5.387$, $CB = (-9.963, -0.8104)$. $q_2 = 18.24$, $CB = (-7.121, 43.6)$. $q_3 = -58.62$, $CB = (-147.7, 30.45)$. $q_4 = 185.5$, $CB = (-105.6, 476.7)$. and $q_5 = -572.2$, $CB = (-1499, 355)$.

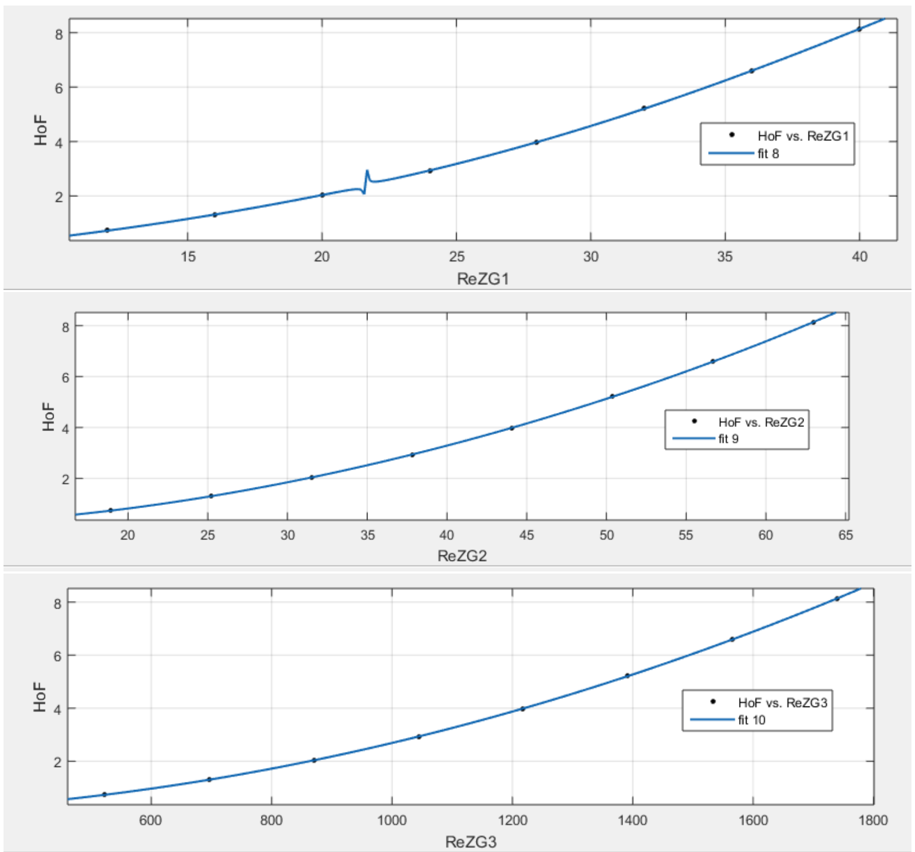


Figure 4.10: (ReZ_1) vs HoF, (ReZ_2) vs HoF and (ReZ_3) vs HoF for HM_n

4.3.3 Models Of Co Indices And Entropies By Using Rational Curve Fitting

We are discussing how we use a method called rational curve fitting to create models for different co indices and entropies. This helps us understand and represent the relationships between these factors in a simple way.

$$E(\overline{M_1}) = \frac{p_1(\overline{M_1})^3 + p_2(\overline{M_1})^2 + p_3(\overline{M_1}) + p_4}{(\overline{M_1})^2 + q_1(\overline{M_1}) + q_2}$$

Where $p_1 = 0.0459$, $CB = (0.02733, 0.06447)$. $p_2 = 3.294$, $CB = (3.189, 3.4)$. $p_3 = 12.23$, $CB = (10.05, 14.41)$. $p_4 = 10.84$, $CB = (7.946, 13.74)$. $q_1 = 4.518$, $CB = (3.767, 5.269)$ and $q_2 = 4.538$, $CB = (3.325, 5.751)$.

$$Entropy(\overline{M_2}) = \frac{p_1(\overline{M_2})^2 + p_2(\overline{M_2}) + p_3}{(\overline{M_2})^2 + q_1(\overline{M_2}) + q_2}$$

Where $p_1 = 3.568$, $CB = (3.48, 3.655)$. $p_2 = 18.05$, $CB = (15.83, 20.26)$. $p_3 = 18.62$, $CB = (15.48, 21.77)$. $q_1 = 6.539$, $CB = (5.777, 7.301)$ and $q_2 = 7.819$, $CB = (6.5, 9.137)$.

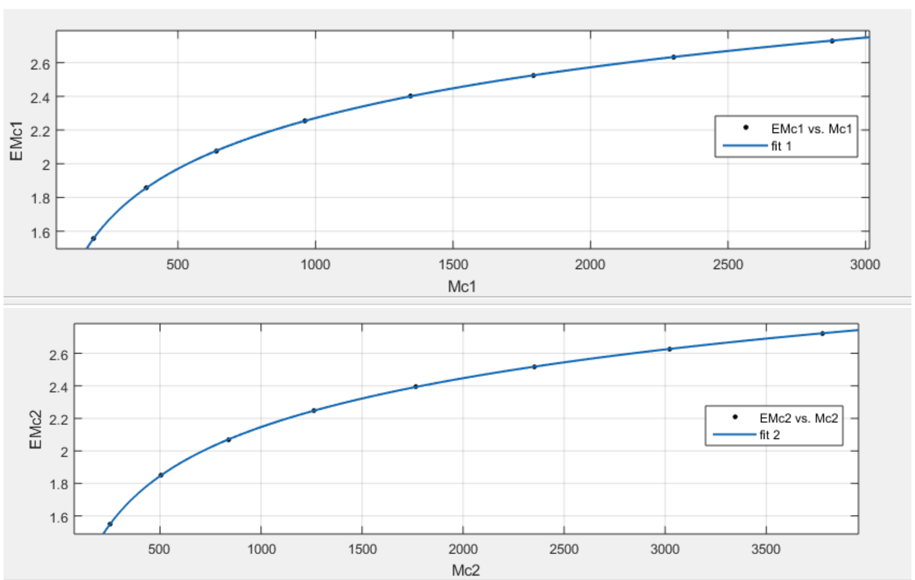


Figure 4.11: $(\overline{M_1})$ vs $(E_{\overline{M_1}})$ and $(\overline{M_2})$ vs $(E_{\overline{M_2}})$ for HM_n

$$E(\overline{HM}) = \frac{p_1(\overline{HM})^3 + p_2(\overline{HM})^2 + p_3(\overline{HM}) + p_4}{(\overline{HM})^3 + q_1(\overline{HM})^2 + q_2(\overline{HM}) + q_3}$$

Where $p_1 = 3.871$, $CB = (-0.5159, 8.258)$. $p_2 = 40.5$, $CB = (-276.7, 357.7)$. $p_3 = 103.8$, $CB = (-1081, 1288)$. $p_4 = 76.51$, $CB = (-978.3, 1131)$, $q_1 = 13.33$, $CB = (-82.99, 109.7)$. $q_2 = 39.27$, $CB = (-399, 477.6)$ and $q_3 = 32.09$ $CB = (-410.3, 474.5)$.

$$E(\overline{F}) = \frac{p_1(\overline{F})^2 + p_2(\overline{F}) + p_3}{(\overline{F})^4 + q_1(\overline{F})^3 + q_2(\overline{F})^2 + q_3(\overline{F}) + q_4}$$

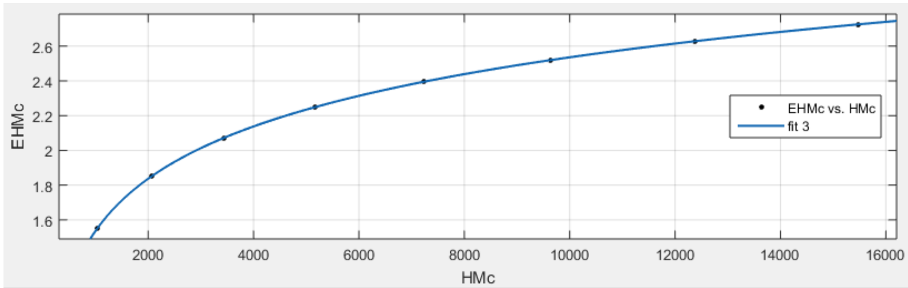


Figure 4.12: $(\overline{HM})$ vs $(E_{\overline{HM}})$ for HM_n

Where $p_1 = 279$, $CB = (-832.3, 1390)$. $p_2 = 386.5$, $CB = (-3396, 4169)$. $p_3 = -34.59$, $CB = (-3616, 3547)$. $q_1 = -4.869$, $CB = (-14.98, 5.244)$. $q_2 = 94.69$, $CB = (-255.1, 444.4)$. $q_3 = 164.1$, $CB = (-1235, 1563)$. and $q_4 = -14.5$, $CB = (-1516, 1487)$.

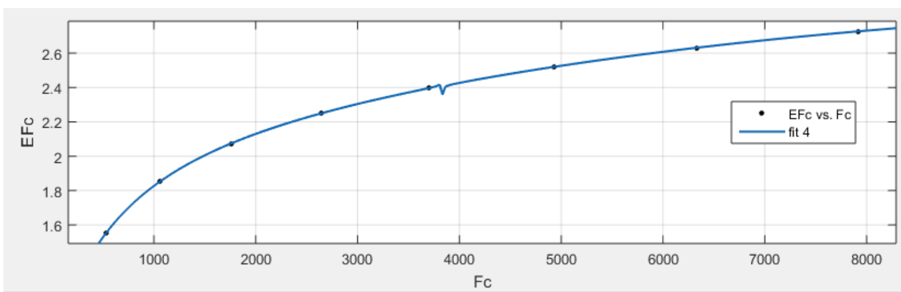


Figure 4.13: $(\overline{F})$ vs $(E_{\overline{F}})$ for HM_n

$$E(\overline{R_{\frac{-1}{2}}}) = \frac{p_1(\overline{R_{\frac{-1}{2}}})^2 + p_2(\overline{R_{\frac{-1}{2}}}) + p_3}{(\overline{R_{\frac{-1}{2}}})^2 + q_1(\overline{R_{\frac{-1}{2}}}) + q_2}$$

Where $p_1 = 3.589$, $CB = (3.502, 3.677)$. $p_2 = 18.79$, $CB = (16.43, 21.15)$. $p_3 = 20$, $CB = (16.53, 23.48)$. $q_1 = 6.751$, $CB = (5.948, 7.555)$ and $q_2 = 8.299$, $CB = (6.859, 9.739)$.

$$E(\overline{R_{-1}}) = \frac{p_1(\overline{R_{-1}})^2 + p_2(\overline{R_{-1}}) + p_3}{(\overline{R_{-1}})^2 + q_1(\overline{R_{-1}}) + q_2}$$

Where $p_1 = 3.567$, $CB = (3.482, 3.652)$. $p_2 = 18$, $CB(15.85, 20.15)$. $p_3 = 18.56$, $CB = (15.52, 21.6)$. $q_1 = 6.52$, $CB = (5.783, 7.258)$ and $q_2 = 7.786$, $CB = (6.51, 9.062)$.

$$E(\overline{R_{\frac{1}{2}}}) = \frac{p_1(\overline{R_{\frac{1}{2}}})^3 + p_2(\overline{R_{\frac{1}{2}}})^2 + p_3(\overline{R_{\frac{1}{2}}}) + p_4}{(\overline{R_{\frac{1}{2}}})^2 + q_1(\overline{R_{\frac{1}{2}}}) + q_2}$$

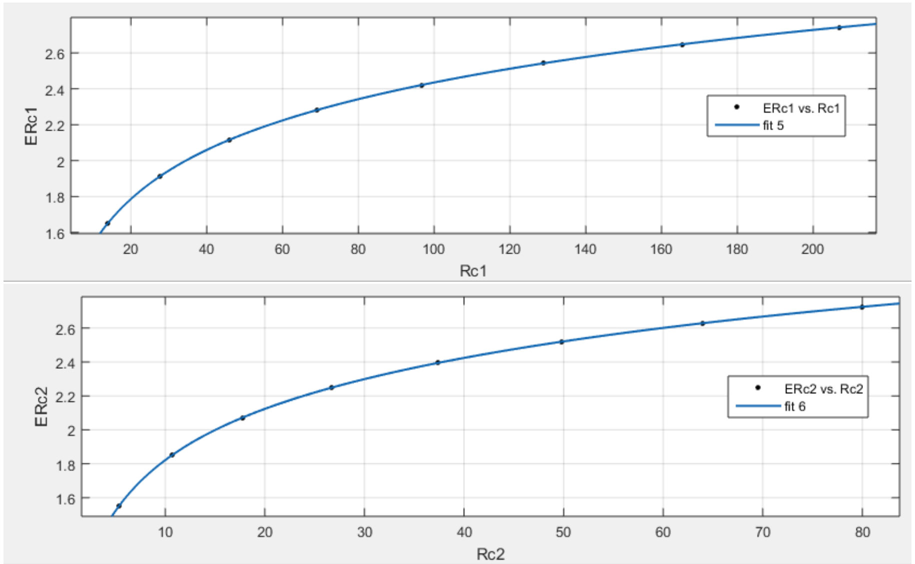


Figure 4.14: $(\overline{R_{\frac{-1}{2}}})$ vs $\left(E_{\overline{R_{\frac{-1}{2}}}}\right)$ and $(\overline{R_{-1}})$ vs $(E_{\overline{R_{-1}}})$ for HM_n

Where $p_1 = 0.0384$, $CB = (0.03372, 0.04309)$. $p_2 = 3.401$, $CB = (3.369, 3.432)$. $p_3 = 14.31$, $CB = (13.5, 15.13)$. $p_4 = 14.07$, $CB = (12.85, 15.28)$. $q_1 = 4.997$, $CB = (4.727, 5.267)$ and $q_2 = 5.419$, $CB = (4.952, 5.886)$.

$$E(\overline{R_1}) = \frac{p_1(\overline{R_1})^3 + p_2(\overline{R_1})^2 + p_3(\overline{R_1}) + p_4}{(\overline{R_1})^2 + q_1(\overline{R_1}) + q_2}$$

Where $p_1 = 0.04409$, $CB = (0.03068, 0.05749)$. $p_2 = 3.303$, $CB = (3.225, 3.381)$. $p_3 = 12.54$, $CB = (10.93, 14.15)$. $p_4 = 11.28$, $CB = (9.135, 13.43)$. $q_1 = 4.637$, $CB = (4.08, 5.194)$ and $q_2 = 4.735$, $CB = (3.834, 5.637)$

$$E(\overline{PM_1}) = \frac{p_1(\overline{PM_1})^3 + p_2(\overline{PM_1})^2 + p_3(\overline{PM_1}) + p_4}{(\overline{PM_1})^3 + q_1(\overline{PM_1})^2 + q_2(\overline{PM_1}) + q_3}$$

Where $p_1 = 7.163$, $CB = (6.585, 7.742)$. $p_2 = 41.78$, $CB = (6.139, 77.41)$. $p_3 = 61.1$, $CB = (-12.83, 135)$. $p_4 = 26.23$, $CB = (-11.5, 63.97)$. $q_1 = 6.578$, $CB = (1.12, 12.04)$. $q_2 = 10.19$, $CB(-2.045, 22.43)$ and $q_3 = 4.547$, $CB = (-1.991, 11.09)$.

$$E(\overline{PM_2}) = \frac{p_1(\overline{PM_2})^3 + p_2(\overline{PM_2})^2 + p_3(\overline{PM_2}) + p_4}{(\overline{PM_2})^3 + q_1(\overline{PM_2})^2 + q_2(\overline{PM_2}) + q_3}$$

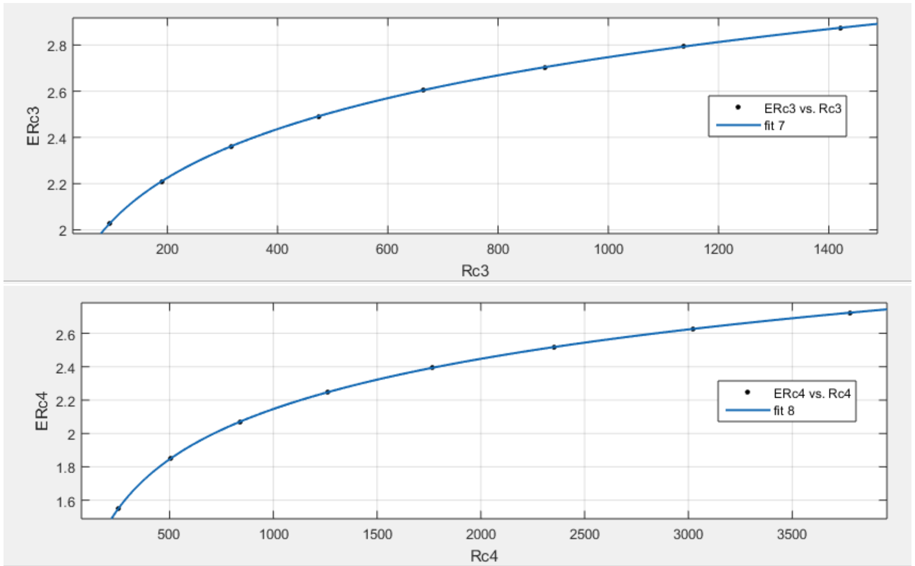


Figure 4.15: $(\overline{R_{\frac{1}{2}}})$ vs $(E_{\overline{R_{\frac{1}{2}}}})$, $(\overline{R_1})$ vs $(E_{\overline{R_1}})$ for HM_n

Where $p_1 = 7.414$, $CB = (6.859, 7.969)$. $p_2 = 43.15$, $CB = (7.667, 78.63)$. $p_3 = 63.07$, $CB = (-10.77, 136.9)$. $p_4 = 27.08$, $CB = (-10.69, 64.85)$. $q_1 = 6.533$, $CB = (1.303, 11.76)$. $q_2 = 10.09$, $CB = (-1.635, 21.82)$ and $q_3 = 4.495$, $CB = (-1.772, 10.76)$.

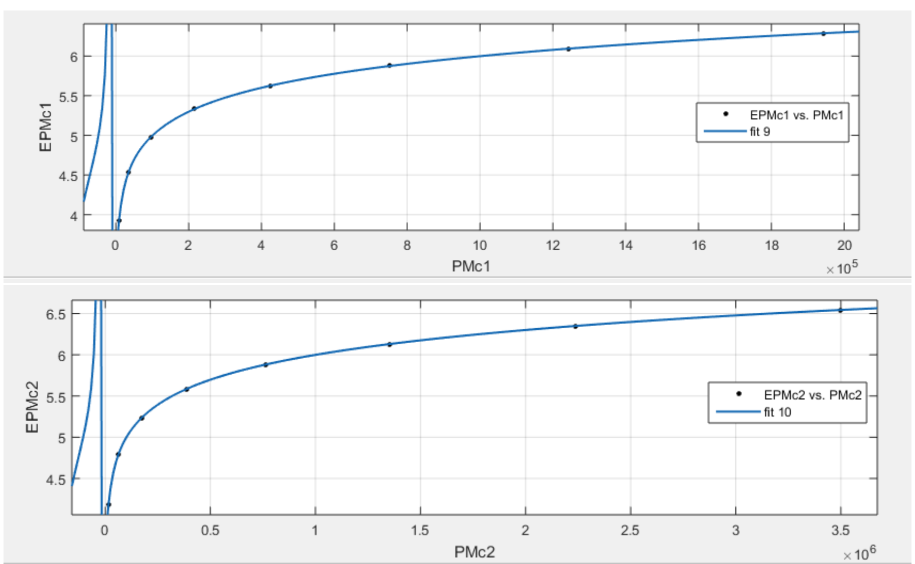


Figure 4.16: $(\overline{PM_1})$ vs $(E_{\overline{PM_1}})$, $(\overline{PM_2})$ vs $(E_{\overline{PM_1}})$ for HM_n

4.3.4 Models Of Co Indices And Heat Of Formation By Using Curve Fitting:

$$HoF(\overline{M_1}) = \frac{p_1(\overline{M_1})^2 + p_2(\overline{M_1}) + p_3}{(\overline{M_1})^2 + q_1(\overline{M_1}) + q_2}$$

Where $p_1 = 701$, $CB = (482.7, 919.3)$. $p_2 = 2417$, $CB = (1569, 3266)$. $p_3 = 2017$, $CB = (1251, 2783)$. $q_1 = 273.1$, $CB = (186.9, 359.3)$ and $q_2 = 516.9$, $CB = (320.7, 713)$

$$HoF(\overline{M_2}) = \frac{p_1(\overline{M_2})^2 + p_2(\overline{M_2}) + p_3}{(\overline{M_2})^2 + q_1(\overline{M_2}) + q_2}$$

Where $p_1 = 698.6$, $CB = (492.3, 905)$. $p_2 = 2400$, $CB = (1601, 3199)$. $p_3 = 1997$, $CB = (1278, 2716)$. $q_1 = 272.1$, $CB = (190.6, 353.5)$ and $q_2 = 511.8$, $CB = (327.6, 696)$.

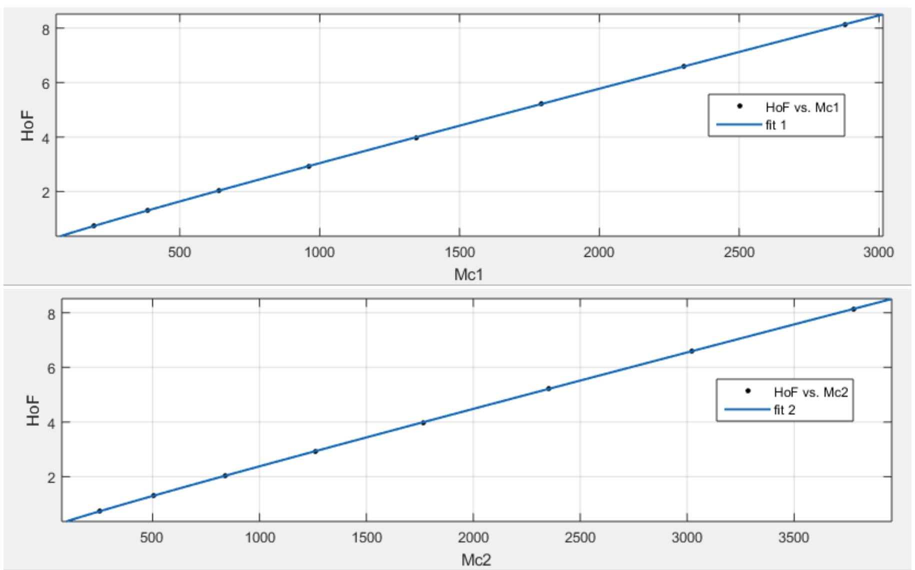


Figure 4.17: $(\overline{M_1})$ vs HoF and $(\overline{M_2})$ vs HoF for HM_n

$$HoF(\overline{HM}) = \frac{p_1(\overline{HM})^2 + p_2(\overline{HM}) + p_3}{(\overline{HM})^4 + q_1(\overline{HM})^3 + q_2(\overline{HM})^2 + q_3(\overline{HM}) + q_4}$$

Where $p_1 = 6382, CB = (-1.266e+05, 1.394e+05).p_2 = 2.005e+04, CB = (-4.19e+05, 4.592e+05).p_3 = 1.558e+04, CB = (-3.393e+05, 3.704e+05).q_1 = -4.846, CB = (-37.85, 28.16).q_2 = 19.85, CB = (-278.8, 318.5).q_3 = 2462, CB = (-4.912e+04, 5.405e+04) and q_4 = 3993, CB = (-8.694e+04, 9.493e+04)$.

$$HoF(\overline{F}) = \frac{p_1(\overline{F})^2 + p_2(\overline{F}) + p_3}{(\overline{F})^4 + q_1(\overline{F})^3 + q_2(\overline{F})^2 + q_3(\overline{F}) + q_4}$$

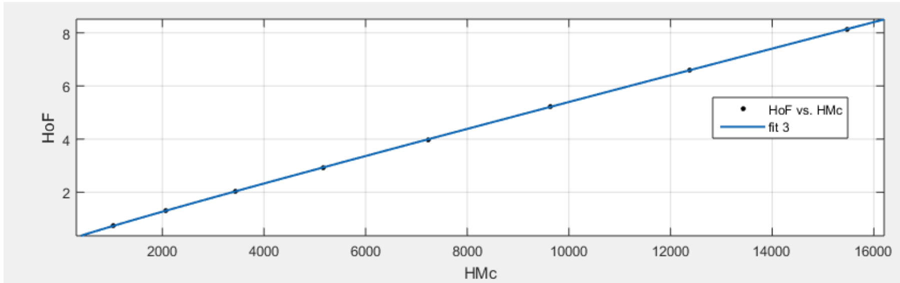


Figure 4.18: $(\overline{HM})$ vs HoF for HM_n

Where $p_1 = -2007$, $CB = (-6.89e+04, 6.489e+04)$. $p_2 = -7288$, $CB = (-2.16e+05, 2.014e+05)$. $p_3 = -6293$, $CB = (-1.678e+05, 1.552e+05)$. $q_1 = -2.16$, $CB = (-44.79, 40.47)$. $q_2 = -1.036$, $CB = (-231.6, 229.5)$. $q_3 = -786.4$, $CB = (-2.658e+04, 2.5e+04)$ and $q_4 = -1613$, $CB = (-4.299e+04, 3.976e+04)$.

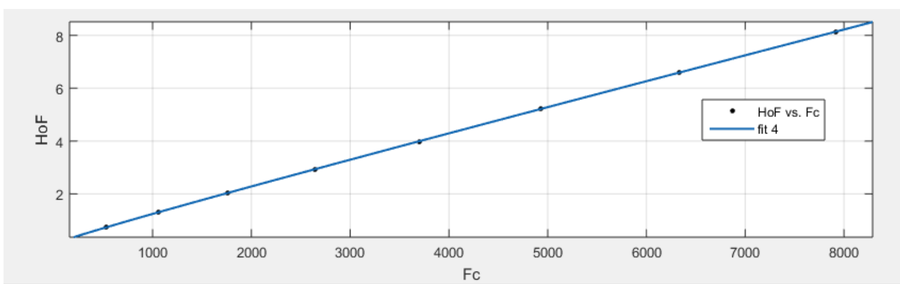


Figure 4.19: $(\overline{F})$ vs HoF for HM_n

$$HoF(\overline{R_{\frac{-1}{2}}}) = \frac{p_1(\overline{R_{\frac{-1}{2}}})^3 + p_2(\overline{R_{\frac{-1}{2}}})^2 + p_3(\overline{R_{\frac{-1}{2}}}) + p_4}{(\overline{R_{\frac{-1}{2}}})^2 + q_1(\overline{R_{\frac{-1}{2}}}) + q_2}$$

Where $p_1 = 2.498$, $CB = (2.484, 2.511)$. $p_2 = 19.49$, $CB = (16.13, 22.84)$. $p_3 = 42.68$, $CB = (31.09, 54.27)$. $p_4 = 28.44$, $CB = (18.79, 38.08)$. $q_1 = 6.053$, $CB = (4.739, 7.366)$ and $q_2 = 7.286$, $CB = (4.814, 9.758)$.

$$HoF(\overline{R_{-1}}) = \frac{p_1(\overline{R_{-1}})^3 + p_2(\overline{R_{-1}})^2 + p_3(\overline{R_{-1}}) + p_4}{(\overline{R_{-1}})^2 + q_1(\overline{R_{-1}}) + q_2}$$

Where $p_1 = 2.508$, $CB = (2.479, 2.538)$. $p_2 = 16.67$, $CB = (9.804, 23.53)$. $p_3 = 32.89$, $CB = (9.441, 56.35)$. $p_4 = 20.27$, $CB = (0.9004, 39.63)$. $q_1 = 4.948$, $CB = (2.263, 7.634)$ and $q_2 = 5.193$, $CB = (0.2302, 10.16)$.

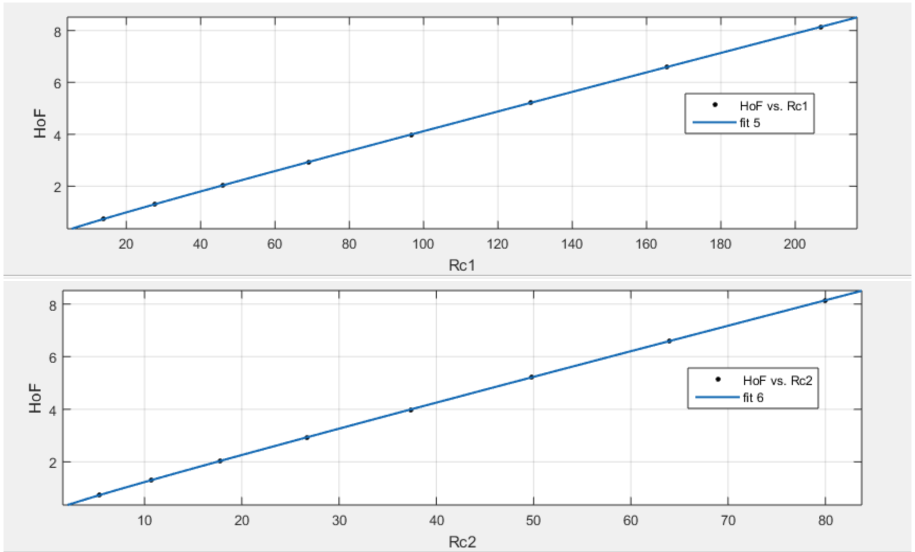


Figure 4.20: $(\overline{R_{\frac{-1}{2}}})$ vs HoF and $(\overline{R_{-1}})$ vs HoF for HM_n

$$HoF(\overline{R_{\frac{1}{2}}}) = \frac{p_1(\overline{R_{\frac{1}{2}}})^2 + p_2(\overline{R_{\frac{1}{2}}}) + p_3}{(\overline{R_{\frac{1}{2}}})^2 + q_1(\overline{R_{\frac{1}{2}}}) + q_2}$$

Where $p_1 = 674$, $CB = (400, 948.1)$. $p_2 = 2324$, $CB = (1253, 3395)$. $p_3 = 1939$, $CB = (968.9, 2909)$. $q_1 = 262.5$, $CB = (154.3, 370.7)$ and $q_2 = 496.8$, $CB = (248.3, 745.3)$.

$$HoF(\overline{R_1}) = \frac{p_1(\overline{R_1})^{+} p_2}{(\overline{R_1})^5 + q_1(\overline{R_1})^4 + q_2(\overline{R_1})^3 + q_3(\overline{R_1})^2 + q_4(\overline{R_1}) + q_5}$$

Where $p_1 = 1843$, $CB = (-5648, 9334)$. $p_2 = 2613$, $CB = (-8037, 1.326e+04)$. $q_1 = -3.46$, $CB = (-8.961, 2.04)$. $q_2 = 5.39$, $CB = (-15.3, 26.08)$. $q_3 = -9.475$, $CB = (-50.07, 31.12)$. $q_4 = 23.37$, $CB(-66.88, 113.6)$ and $q_5 = 669.6$, $CB = (-2060, 3399)$.

$$HoF(\overline{PM_1}) = \frac{p_1(\overline{PM_1})^3 + p_2(\overline{PM_1})^2 + p_3(\overline{PM_1}) + p_4}{(\overline{PM_1})^2 + q_1(\overline{PM_1}) + q_2}$$

Where $p_1 = 1.016$, $CB = (0.7663, 1.266)$. $p_2 = 10.71$, $CB = (9.25, 12.17)$. $p_3 = 18.63$, $CB = (13.47, 23.79)$. $p_4 = 8.763$, $CB = (5.529, 12)$. $q_1 = 2.972$, $CB = (2.25, 3.695)$ and $q_2 = 1.882$, $CB = (1.182, 2.582)$.

$$HoF(\overline{PM_2}) = \frac{p_1(\overline{PM_2})^3 + p_2(\overline{PM_2})^2 + p_3(\overline{PM_2}) + p_4}{(\overline{PM_2})^2 + q_1(\overline{PM_2}) + q_2}$$

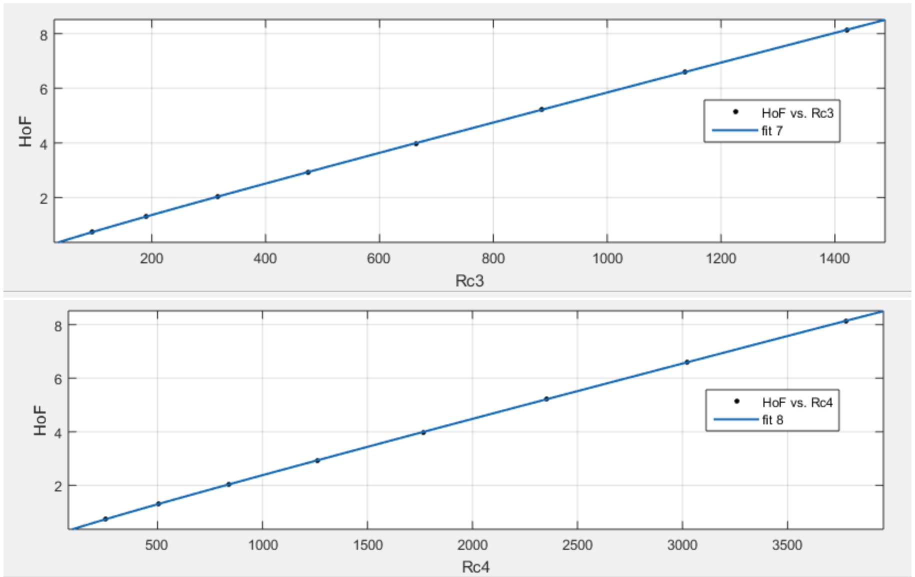


Figure 4.21: $(\overline{R_{\frac{1}{2}}})$ vs HoF, $(\overline{R_1})$ vs HoF for HM_n

Where $p_1 = 1.016$, $CB = (0.7661, 1.266)$. $p_2 = 10.71$, $CB = (9.25, 12.17)$. $p_3 = 18.63$, $CB = (13.47, 23.8)$. $p_4 = 8.765$, $CB = (5.529, 12)$. $q_1 = 2.972$, $CB = (2.25, 3.695)$ and $q_2 = 1.882$, $CB = (1.182, 2.583)$.

At this point, we have finished our research on the topological description of the Mobius

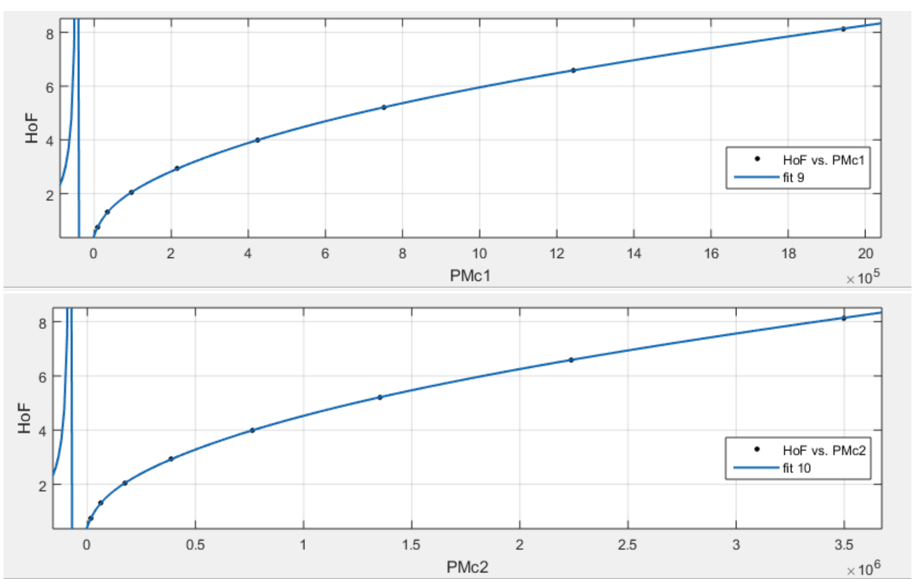


Figure 4.22: $(\overline{PM_1})$ vs HoF, $(\overline{PM_2})$ vs HoF for HM_n

strip through the use of degree based indices and co indices.

Chapter 5
Conclusion

We found a strong connection between certain topological indices (entropies), co indices (entropies) and heat of formation in our study for HM_n. We used a tool called Rational Curve Fitting in MATLAB to do this. We paid a lot of attention to two specific indices, Redefined Zagreb and K Banhatti, and three specific co-indices, Zagreb, Randic and Forgotten, and checked how closely they are related to their entropies/HoF. To make it easier to understand, we also looked at pictures and graphs of these indices and co indices and how they connect to entropies/HoF. By doing all this with Matlab, we could see patterns and connections between indices and their entropies/HoF, co indices and their entropies/HoF. Our discoveries provide us with a clear understanding of relationship within particular system.

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