Chemical Trees with Extermal Sombor Index Among Chemical Trees with Given Order and Number of Vertices of Maximum Degree

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2023

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I dedicate this thesis to my loving parents, venerable supervisor, respectable teachers and fellows for their limitless support and encouragement.

Acknowledgement

Primarily I would like to express my utmost gratitude to Allah, the ultimate source of wisdom and blessings, for His consistent counsel and aid throughout my journey. I extend my heartfelt gratitude to the Prophet Muhammad (peace be upon him) for his profound teachings, which is a perpetual source of enlightenment.

I am grateful to principal of SNS, my supervisor, Prof. Rashid Farooq, for his exceptional guidance, expertise, and unwavering support. His invaluable insights, critical evaluation and constructive feedback have significantly shaped the outcome of this thesis. I also want to acknowledge the contribution of the members of the (GEC) for their time and involvement during the evaluation process.

Furthermore, I express my sincere appreciation to the committed staff members at (SNS) for their tremendous assistance, cooperation and for fostering a conducive research environment. I would also like to extend my gratitude to NUST for providing me with a platform for exploring great learning opportunities and interactions with fellow students, that have greatly enhanced my understanding.

My heartfelt thanks to my seniors for their advice and wisdom, which have been instrumental in shaping my research approach. I am also indebted to my friends for their encouragement, and camaraderie throughout this challenging journey. Their presence and stimulating discussions have provided ongoing inspiration and motivation.

Finally, I would like to express my profound appreciation to my family for their unconditional love, unflinching belief in my abilities, and unending support. Their encouragement, sacrifices, and steadfast trust in my potential have been the driving force behind my perseverance and success in this achievement.

Iqra Jahangir

Abstract

Gutman and Trinajstic proposed the notion of a degree-based index in 1972. Topological indices based on vertex degree play a significant role in graph theory by capturing important structural information about graphs, connectivity and centrality measures, and the identification of influential vertices. These are also valuable in graph classification tasks and network modeling, assisting in the categorization of graphs and the comprehension of real-world networks.

One of those vertex based topological indices namely Sombor index was introduced by Gutman in 2020. Being a relatively nascent field, Sombor index has captured the interest of researchers, driving it to become an essential concept in the field of chemical graph theory.

In this work, we find a chemical tree with maximum Sombor index amoung the class of chemical trees with the fixed number of vertices of maximum degree. Similarly, we find a chemical tree with minimum Sombor index amoung the class of chemical trees with the fixed number of vertices of maximum degree.

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Chapter 1

Introduction to graph theory

This chapter is concerned with the basic concepts and definitions associated with graph theory. Recently, graph theory has emerged as a significant mathematical tool. It is a field of study that examines the properties and relationships of graphs, which consist of vertices connected by edges. It is an essential tool in numerous disciplines, including computer science, mathematics, and network analysis. Graph theory encompasses multiple domains, such as connectivity, paths, cycles, planarity, graph coloring, chemical, spectral and algebraic graph theory each examining particular aspects of graphs and their characteristics. Graph theory enables us to acquire insights into complex systems, optimize network designs, and address issues in a variety of disciplines by researching these branches.

1.1 Origin and evolution of graph theory

The work of Swiss mathematician Leonhard Euler in the 18th century established graph theory as a mathematical field. In 1736, Euler addressed the "Seven Bridges of Königsberg" problem [1], which involved finding a path through the city namely Königsberg that would cross all of its seven bridges only once, ultimately returning to the starting point. Euler used the notion of a "graph" to describe Königsberg's land masses (vertices) and bridges (edges), allowing him to deal with the problem mathematically.

Following Euler's groundbreaking contributions, other mathematicians further progressed the field of graph theory. Augustin-Louis Cauchy, a French mathematician, made fundamental contributions to graph theory in the early 19th century by exploring planar graphs.

Later, in the 20th century, the discipline of graph theory gained more prominence and observed major developments. Pioneers like Frank Harary, Paul Erdős, and William Tutte made key contributions to graph theory in areas like connectivity, graph coloring and graph algorithms. Their work broadened the scope of graph theory, making it a major area of study. The ongoing research and exploring of graph theory continue to uncover new insights and applications, making it an influential and continually evolving field of study.

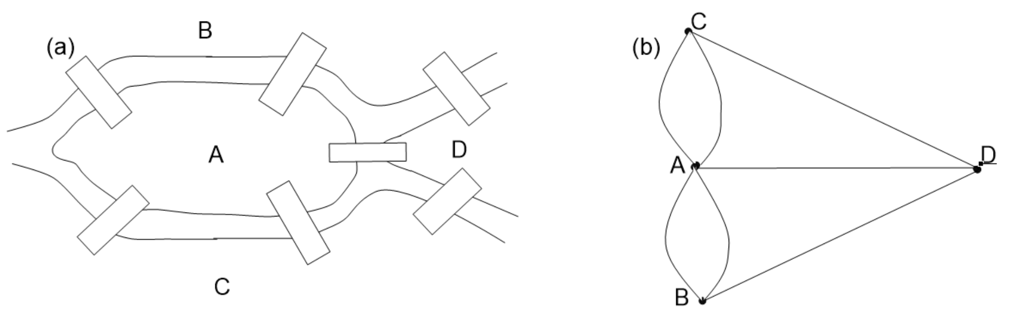

Figure 1.1: (a) Königsberg seven bridge problem (b) Graphical representation

1.2 Introduction and representation of graphs

In this section, we give well known definitions of graph theory.

1.2.1 Graphs and some basic definitions

A *graph* is a fundamental structure, mathematically used to represent relationships between objects. It is made up of three components: vertices, edges and incidence function. *Edges* or edge set is represented by $E(G)$ and it signify links or interactions between pairs of vertices, whereas *vertices* (also called nodes) or vertex set is represented by $V(G)$ and it represent distinct things. The *incidence function* I_G maps each edge into a pair of vertices. An edge between vertex v_i and v_j is represented by ij. The *order* of a graph refers to the total number of vertices it consists of and denoted by n or $V(G)$, whereas the total number of edges is referred as *size* of graph denoted by m. In Figure 1.1 $n = 4$ and $m = 7$.

Incident edges on a vertex are the edges that are directly connected to it. *Degree* of vertex is the number of edges incident to it and is denoted by $deg(v)$. Edges between the same pair of vertices are *multiple edges* and *loops* are edges that has sane starting and ending vertex, making a self-connection. In Figure 1.1 (b), vertices A and B, A and C have multiple edges. *Adjacent vertices* are those vertices that are end points of an edge, whereas *non-adjacent vertices* do not have an edge between them. *Neighbors* of a vertex are its adjacent vertices and are denoted by $N(v)$, as in Figure 1.1, $N(C) = \{A, D\}$.

A *connected graph* has a path between any pair of vertices, ensuring that each vertex is reachable from any other vertex. In contrast, a *disconnected graph* consists of multiple components, indicating there are at least two vertices that have no path between them. *Components* of a graph are the maximal connected subgraphs. A graph whose vertices and edges are subset of another graph is called a *subgraph*. A *maximal connected subgraph* is one to which no vertex can be added without breaking its connectedness. A *pendant vertex* is also known as a *leaf* and has degree 1, whereas *isolated vertex* has degree 0. A *simple graph* is one with no multiple edges or loops. In a graph, *clique* is a set of vertices that are pairwise adjacent, while *independent set* a set of vertices that are pairwise non-adjacent.

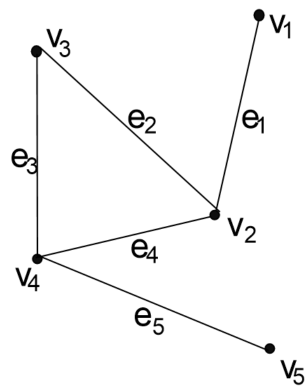

Figure 1.2: Simple graph

Two graphs $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ and $\mathcal{G}_1 = (\mathcal{V}_1, \mathcal{E}_1)$, if there exist bijections $\phi : \mathcal{V} \to \mathcal{V}_1$ and $\psi : \mathcal{E} \to \mathcal{E}_1$, that preserve the endpoint relations of $\mathcal{G}$ and $\mathcal{G}_1$ are said to be isomorphic that is, if $v_i \in \mathcal{V}$ is an endpoint of $e_i \in \mathcal{E}$ then $\phi(v_i) \in \mathcal{V}_1$ is an endpoint of $\psi(e_i) \in \mathcal{E}_1$ denoted by $\mathcal{G} \cong \mathcal{G}_1$. Apparently *Isomorphic graphs* must have equal number of vertices of each degree, same number of vertices and edges but these conditions are not sufficient for graphs to be called isomorphic to each other. Isomorphic graphs exhibit same fundamental structure, have similar connection patterns, retaining vertices associations. This indicates that any traits or characteristics that apply to one graph apply to its isomorphic counterpart.

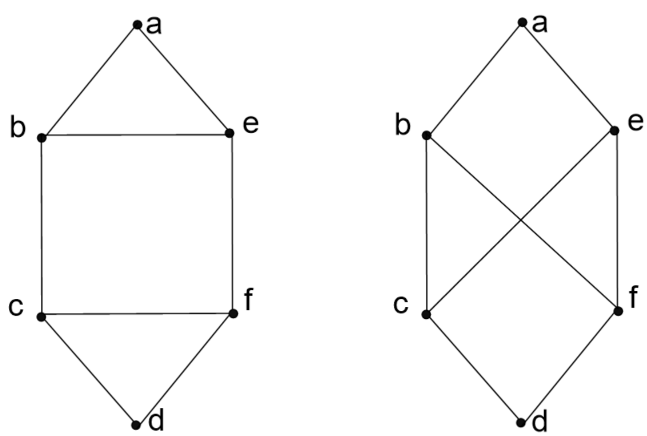

Figure 1.3: Isomorphic graphs

1.2.2 Graph representation

There are several ways of graph representations, one of them is matrix representation. Matrix representation is widely used to store graphic data. Now we will discuss two types of matrix representation

A square matrix that depicts the relationships between vertices in a graph is known as an *adjacency matrix*. Adjacency matrix is denoted by $A(G) = [a_{ij}]$, in which a_{ij} is the number of edges in G with endpoints v_i and v_j and is defined as

$$a_{ij} = \begin{cases} 1, & \text{if there is an edge between vertex } v_i \text{ and } v_j \\ 0, & \text{otherwise.} \end{cases}$$

Adjacency matrix for the graph in Figure 1.2 is,

$$A(G) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

An *incidence matrix* is a graph representation that uses rows to represent vertices and columns to represent edges. Incidence matrix is denoted by $M(G) = [m_{ij}]$, in which m_{ij} is defined as

$$m_{ij} = \begin{cases} 1, & \text{if } v_i \text{ is an endpoint of } e_j \\ 0, & \text{otherwise.} \end{cases}$$

Incidence matrix for the graph in Figure 1.2 is,

$$M(G) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

1.3 Fundamental concepts related to graphs

In this section, we furnish fundamental concepts related to graphs.

1.3.1 Graph structures

Graph structures are essential elements that form the building blocks of graph theory. They describe the connections and relationships between vertices and edges, allowing us to study and analyze graph characteristics and behavior. Few are discussed next.

A *walk* in a graph, is an alternating sequence $v_0, e_1, v_1, e_2, v_2, \ldots, v_{n-1}, e_n, v_n$ of vertices and edges, such that $e_i = v_{i-1}v_i$. It symbolizes a journey or traversal across the graph, with each step moving from one vertex to an adjacent vertex connected by an edge. Walks can be closed or open depending on whether their starting and end points are same or different respectively. A *path* is a simple graph of sequence $v_0, e_1, v_1, e_2, v_2, \ldots, v_{n-1}, e_n, v_n$ such that, $e_i = v_{i-1}v_i$ and $v_i \neq v_j$ for all $i, j \in V(G)$. *Length* of a path is number of edges in it and path of n vertices is denoted by P_n. *Trail* is a walk that allows repetition of vertices while ensuring that each edge is only appears once. A trail is closed if its first and last vertex are the same. A *circuit* is a closed trail. *Cycle* is a trail where only starting and ending vertices are repeated. A cycle of length n is denoted by C_n.

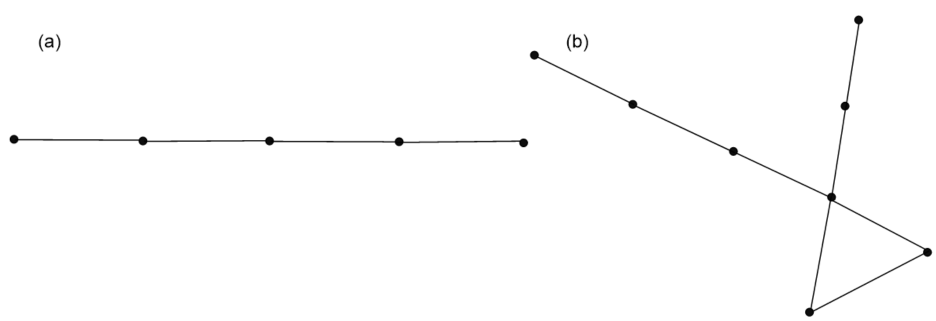

Figure 1.4: (a) Open walk, path P_5 (b) Closed walk, trail

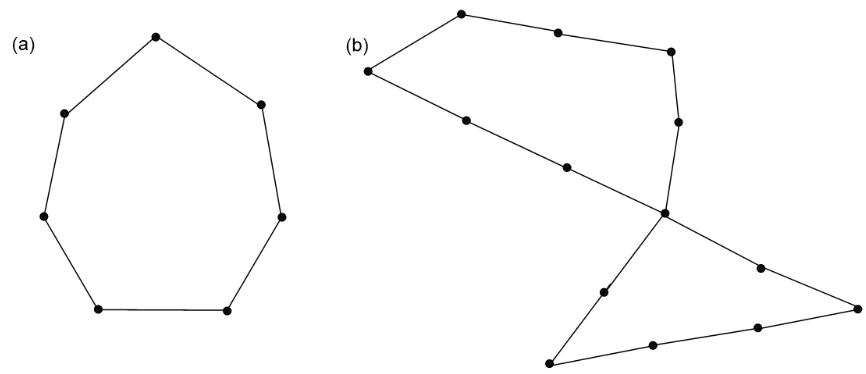

Figure 1.5: (a) Cycle C_5 (b) Circuit

Trees are another important graph structure first studied by Cayley in 1857 [2]. A tree is a connected graph, in which every pair of vertices have exactly one path between them. That is, a tree is connected graph that contains no cycle. Trees are commonly used to depict hierarchical connections or organized data structures, and their features allow fast searching and sorting algorithms to be implemented.

1.3.2 The first theorem of graph theory

Theorem 1.3.1. [3](Handshaking Lemma) *If $\mathcal{G}$ is any graph with edge set $\mathcal{E}(\mathcal{G})$, then*

$$\sum_{v \in \mathcal{V}(\mathcal{G})} deg(v) = 2\mathcal{E}(\mathcal{G}).$$

1.3.3 Graph metrices

Graph metrices are quantitative measures that give useful information about a graph's basic characteristics and attributes. Some of these are discussed next.

In a graph, the length of shortest path between a pair of vertices is *distance* between them. Distance between a vertex v_x and another vertex v_y is denoted by $d(v_x, v_y)$. A graph's *diameter* is denoted by diam(G) and is defined as

$$\text{diam}(G) = \max\{d(v_x, v_y) \mid v_x, v_y \in V(G)\}.$$

The *eccentricity* calculates how distant a vertex is from the graph's furthest vertex. Eccentricity of some vertex v_x denoted by $e(v_x)$ is mathematically defined as

$$e(v_x) = \max\{d(v_x, v_w) \mid v_w \in V(G)\}.$$

The *radius* of a graph represented by rad(G) defined as

$$rad(G) = \min\{e(v_x) \mid v_x \in V(G)\}.$$

Center of a graph is denoted by $C(G)$ and mathematically defined as

$$C(G) = \{v_x \in V(G) \mid e(v_x) = \text{rad}(G)\}.$$

1.3.4 Graph operations

A *cut-edge*, also known as a *bridge*, is a graph edge that, if deleted, would increase the number of components in that graph. If e is an edge that is removed from graph $\mathcal{G}$ then the resulting graph is denoted by $\mathcal{G} - e$. In Figure 1.2, e_1 and e_5 are cut-edges.

A *cut-vertex*, is such a vertex in a graph that removing it, would increase the number of components. In Figure 1.2, v_2 and v_4 are cut-vertices.

1.3.5 Extremal graphs

In graph theory, *extremal graphs* are graphs that have specific properties or characteristics that make them distinctive or optimal within a particular class of graphs. The study of extremal graphs focuses on discovering maximum and minimum values of graph parameters under particular limitations or circumstances. Mantel [5] and Paul Turan [6] worked for the advancement of extremal graph theory.

1.4 Some special graphs

Graphs are classified into numerous categories depending on their features and properties in graph theory. An *undirected graph* has edges that have no direction or orientation. The edges reflect symmetric interactions between vertices, thus moving from one vertex to another via the edges is feasible in both directions. While, A *directed graph*, also known as a *digraph*, is a graph with edges that have a defined direction or orientation. The edges are shown by arrows, demonstrating the direction of vertices. A *weighted graph* is one in which every edge has a numerical number or weight given to it. These weights indicate a numerical quantity such as distance, cost or capacity. A graph whose vertices can be divided into two disjoint independent sets in G and union is $V(G)$ *bipartite graph.* If there is an edge connecting each pair of vertices, the graph is *complete..* K_n denotes a complete graph with n vertices. A *complete bipartite graph* is one in which the vertices may be divided into two subsets not having an edge between vertices of same subset and their must be edge between vertices of different subsets. It is written as K_{n_i,n_j}, where n_i and n_j are the number of vertices in each independent set.

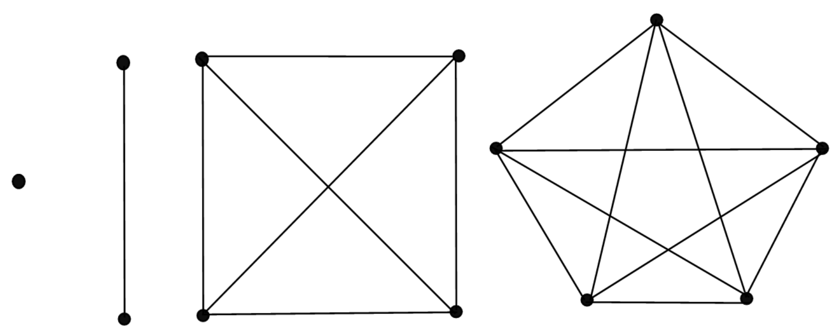

Figure 1.6: Complete graphs: $\mathcal{K}_1, \mathcal{K}_2, \mathcal{K}_4$ and $\mathcal{K}_5$

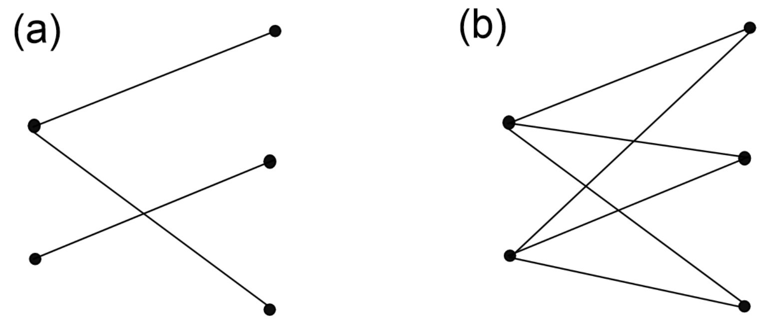

Figure 1.7: (a) Bipartite graph (b) Complete bipartite graph $K_{2,3}$

A *pseudograph* is a graph with multiple edges and loops. A *regular graph* is such a graph in which all of the vertex degrees are the same. A *k-regular graph* is one with every vertex having a degree k. An *infinite graph* is one with an infinite number of vertices or edges. An *empty graph*, is a graph where there is no edge between all the vertices. An *null graph* is one that contains no vertices and edges. An *Eulerian graph* contains an *Eulerian cycle*, which is a cycle that visits each edge precisely once. In Eulerian graph, degree of each vertex is even.

A *broom* graph is a tree that consists of a path and all the pendant vertices are attached on one end of that path. A *rooted tree* is a tree that has one vertex identified as the root vertex. A *caterpillar* is a tree in which a path is formed by deleting all of the leaf vertices. *Chemical tree* T is a tree satisfying $d_T(v) \leq 4$ for each $v \in V(T)$.

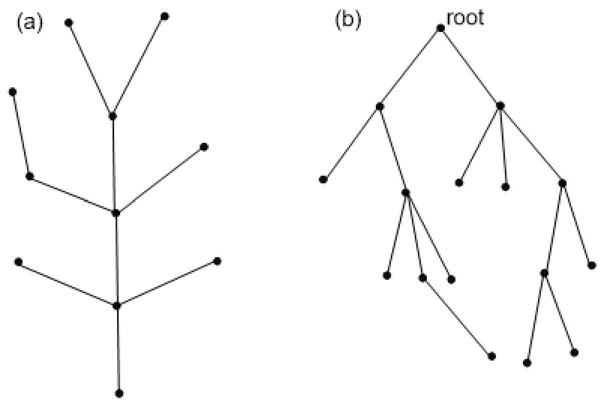

Figure 1.8: (a) Tree (b) Rooted tree

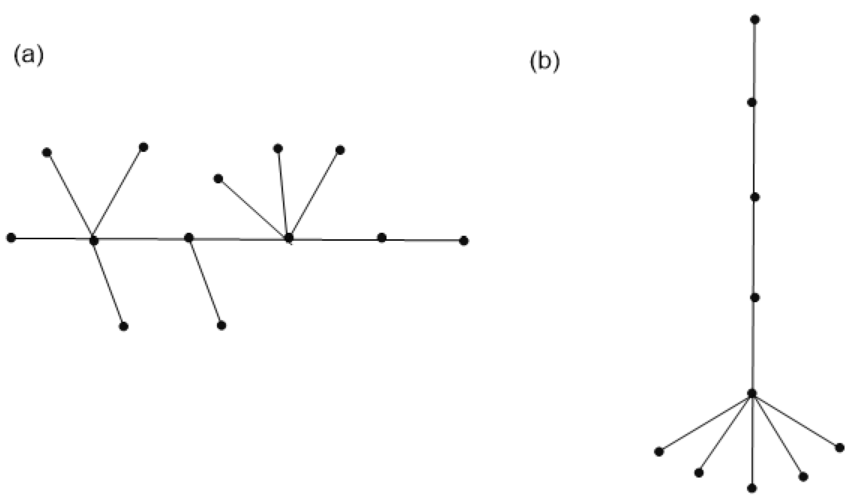

Figure 1.9: (a) Caterpillar (b) Broom

1.5 Chemical graph theory

Chemical graph theory is a field of graph theory concerned with the mathematical modelling, study of molecular structures and chemical reactions. Sylvester [4] and Cayley [2] were pioneers of introducing chemical graphs in mathematics literature. It gives a framework for comprehending the interactions between atoms, bonds and molecules using graph theory concepts like vertices (atoms) and edges (bonds). Researchers can get insights into numerous elements of chemical systems, such as molecular structure [12], reactivity, and characteristics, by employing graph theory methodologies [13]. Some fundamental topics and techniques in chemical graph theory are as follows:

(i) Molecules structures are represented as graphs, with vertices as atoms and edges as bonds. Depending on whether the bonds have a definite orientation or not, the graph can be either directed or undirected.

(ii) Molecular descriptors are quantitative metrics that capture numerous properties of a molecule. Graph invariants or other mathematical procedures can be used to determine them from the graph representation.

(iii) Symmetry in chemical systems is significant because it determines the physical and chemical characteristics of molecules. Graph theory provides techniques for analyzing molecular graph symmetry and calculating symmetry groups.

(iv) Topological indices are numerical numbers that are generated from graph invariants and are used to characterize molecule structures as well as predict attributes like boiling point, stability and biological activity.

(v) Chemical graph theory may also be applied to the study of chemical processes. Graph algorithms can be used to analyze chemical reaction paths, rates, and other features.

(vi) Quantitative structure-activity relationship QSAR and structure-property relationship QSPR models are used to predict a molecule's activity or characteristics based on structural factors [15, 14].

(vii) In chemical graph theory, several graph algorithms are used to tackle specific issues. These methods allow researchers to effectively analyse enormous chemical databases, search for comparable compounds, and explore chemical space.

Chapter 2

Topological indices and known results

Topological indices are numerical parameters obtained from molecular graph of a chemical compound. In 1947, Harry Wiener [7] introduced and used it to compare the boiling temperatures of several alkane isomers. Since then chemical data bases has recorded over 3000 topological graph indices. Topological indices were further developed in early 1970s [10, 11].

Topological indices provide quantitative measures of the molecular structure and are used to correlate structural features with various properties of interest, such as boiling point, viscosity, toxicity and biological activity. In chemo informatics, drug discovery, and computational chemistry, topological indices are commonly used. Topological indices are graph invariants, which means they are independent of the individual atom or bond labelling and rely entirely on the topology of the molecular graph. They extract structural information from the graph. Topological indices may be computed through the use of mathematical formulae or algorithms. Topological indices are interesting because they can capture crucial structure properties without explicitly considering atom spatial arrangement. Topological indices are now computationally efficient and broadly applicable, allowing researchers to make predictions and correlations based only on molecular connection. Further Applications of topological indices are provided in [8, 9].

2.1 Classes of topological indices

There are two main classes of topological indices which are:

(i) Topological indices w.r.t. distances.

(ii) Topological indices w.r.t. degrees.

2.1.1 Topological indices w.r.t. distances

Harold Wiener initially proposed distance-based topological indices in 1947 [7], particularly the Wiener index. Distance-based topological indices assess the topological properties of a molecular network using the distances between atoms. The distance between two atoms is defined as the minimum amount of bonds or edges required to join them.

Different distance-based topological indices capture different aspects of molecular structure. The Wiener index, for example, is defined as the sum of all pairwise distances between atoms in a molecular network. It calculates the total molecule size and branching. Other distance-based indices, including Balaban index, concentrate on specific distance connections and connectivity patterns in the molecular network. Here is a simplified distance-based topological indices representation,

$$\text{Distance based index} = f(d_1, d_2, ..., d_n).$$

Here, f denotes a mathematical function or operation that combines the distances and $d_1, d_2, ..., d_n$ are the distances in between pairs of atoms in the molecular graph.

Researchers may extract quantitative descriptors that correspond with numerous physio-chemical features, such as boiling temperatures, melting points and bio-activity, by computing distance-based topological indices. These indices give useful insights into chemical compound structure-property interactions, assisting in the creation and optimization of medications, materials, and other chemical substances. Some of the topological indices w.r.t. distances are listed in Table 2.1, where m and n are total number of edges and vertices in a graph G respectively.

Names of indices	Mathematical formulas	References
Wiener index	$\sum_{v,w\in\mathcal{V}(G)} d_G(v,w)$	[7]
Platt number	$\sum_{i=1}^{m} d(e_i)$	[22]
Szeged index	$\sum_{vw\in\mathcal{E}(G)} n_v(vw)n_u(vw)$	[28]
Hyper-Wiener index	$\frac{1}{2}\sum_{w\subseteq V(G)}\sum_{v\subseteq V(G)}[d_G(w,v)+(d_G(w,v))^2]$	[21]
Balaban index	$\frac{m}{\gamma+1}\sum_{wv\in\mathcal{E}(G)}\frac{1}{\sqrt{\sigma_G(w)\sigma_G(u)}}$; $\gamma=m-n+c, \sigma_G(u)=\sum_{w\in\mathcal{V}(G)} d_G(u,w)$, c=constant	[17]
Schultz index	$\frac{1}{2}\sum_{w,v\in V(G)}(d_w+d_v)d_G(w,v)$	[29]
Gordon-Scantlebury index	$\frac{\sum_{w\in V(G)}(d_v)^2}{2}-\|m\|$	[25]
Non-self-centrality number	$\sum_{x\neq z}\|\epsilon(x)-\epsilon(z)\|$; $\epsilon(x)=max\{d_G(x,z)\mid z\in V(G)\}$	[27]
Harary number	$\frac{1}{2}\sum_{w,v\in V(G)}\frac{1}{d_G(w,v)}$	[30]
Balaban centric index	$\sum_{g=1}^{R} n_g^2$	[18]
Average eccentricity index	$\frac{1}{n}\sum_{z\in V(G)}\epsilon(z)$; $\epsilon(z)=max\{d_G(z,w)\mid\forall w\in V(G)\}$	[24]
Total eccentricity index	$\sum_{z\in V(G)}\epsilon(z)$; $\epsilon(z)=max\{d_G(z,w)\mid\forall w\in V(G)\}$	[19]
Eccentricity based geometric-arithmetic	$\sum_{zw\in E(G)}\frac{2\sqrt{\epsilon(z).\epsilon(w)}}{\epsilon(z)+\epsilon(w)}$; $\epsilon(z)=max\{d_G(z,v)\mid\forall v\in V(G)\}$	[20]
Zagreb eccentricity index	$\sum_{zw\in E(G)}[\epsilon(z)+\epsilon(w)]$; $\epsilon(z)=max\{d_G(z,v)\mid\forall v\in V(G)\}$	[23, 26]
Eccentric distance sum	$\sum_{z\in\mathcal{V}(G)}\sum_{w\in\mathcal{G}V(G)}\epsilon(w)d_G(z,w)$; $\epsilon(w)=max\{d_G(w,v)\mid\forall v\in V(G)\}$	[31]

Table 2.1: Topological indices w.r.t. distances

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2.1.2 Topological indices w.r.t. degrees

Gutman and Trinajstic established and extended degree-based topological indicies such as Zagreb indices in 1972 [10], which have been used for over 50 years. A set of mathematical descriptors known as degree-based topological indices is used to characterise the structural features of graphs or molecules. These indices are determined by the number of vertices in the graph or the chemical structure. Here is a simplified Topological indices w.r.t. degrees representation,

$$\text{Degree based index} = \sum_{xy\in E(G)}(d_G(x), d_G(y)) = \sum_{xy\in E(G)}(d_G(y), d_G(x)).$$

Here, f denotes a mathematical function that is symmetric and combines the degrees.

Because of their computational efficiency, degree-based indices have been extensively studied and used. They obtain crucial structural information about graphs or molecules and can be employed in QSAR research, chemical similarity analysis, or graph theory applications. By reflecting the effect of local connection patterns, these indices provide insights into molecular attributes like as boiling temperatures, toxicity, or biological activities.

There have been several more degree-based indexes developed, each concentrating on a different feature of graph or molecule structure. Specific vertex degrees, degree sequences, or combinations of degrees and other structural features may be considered by these indices. Some of these indices are mentioned in Table 2.2.

Names of indices	Mathematical formulas	References
First Zargeb index	$\sum_{z\in\mathcal{V}(\mathcal{G})} d_z^2(\mathcal{G}) = \sum_{zw\in\mathcal{E}(\mathcal{G})} d_z(\mathcal{G}) + d_w(\mathcal{G})$	[10]
Second Zargeb index	$\sum_{zw\in\mathcal{E}(\mathcal{G})}(d_z(\mathcal{G}))(d_w(\mathcal{G}))$	[10]
Randić index	$\sum_{wz\in\mathcal{E}(\mathcal{G})} \frac{1}{\sqrt{(d_w(\mathcal{G}))(d_z(\mathcal{G}))}}$	[21]
Atom-bond connectivity index	$\sqrt{\frac{d_u(\mathcal{G}) + d_G v(\mathcal{G}) - 2}{(d_u(\mathcal{G}))(d_v(\mathcal{G}))}}$	[34]
Harmonic index	$\frac{2}{d_u(\mathcal{G}) + d_v(\mathcal{G})}$	[36, 40]
Sum connectivity index	$\frac{1}{\sqrt{d_u(\mathcal{G}) + d_v(\mathcal{G})}}$	[39]
Augmented Zagreb index	$\left[\frac{(d_u(\mathcal{G}))(d_v(\mathcal{G}))}{d_u(\mathcal{G}) + d_v(\mathcal{G}) - 2}\right]^3$	[37]
Geometric-arithmetic index	$\frac{\sqrt{(d_u(\mathcal{G}))(d_v(\mathcal{G}))}}{\frac{1}{2}[d_u(\mathcal{G}) + d_v(\mathcal{G})]}$	[35]
Sigma index	$\sum_{uv\in\mathcal{E}(\mathcal{G})}(d_u(\mathcal{G}) - d_v(\mathcal{G}))^2$	[38]
Hyper Zargeb index	$\sum_{uv\in\mathcal{E}(\mathcal{G})}(d_u(\mathcal{G}) + d_v(\mathcal{G}))^2$	[33]
Hyper Zargeb coindex	$\sum_{uv\in\mathcal{E}(\mathcal{G})}(d_u(\mathcal{G}) d_v(\mathcal{G}))^2$	[38]
Inverse degree index	$\sum_{vw\in\mathcal{E}(\mathcal{G})} \frac{(d_v(\mathcal{G}))^2 + (d_w(\mathcal{G}))^2}{(d_v(\mathcal{G}))^2(d_w(\mathcal{G}))^2}$	[37]
Forgotten index	$\sum_{x\in\mathcal{V}(\mathcal{G})} d_x^3(\mathcal{G})$	[41]
Forgotten coindex	$\sum_{wv\in\mathcal{E}(\mathcal{G})}[(d_w(\mathcal{G}))^2 + (d_v(\mathcal{G}))^2]$	[42]
Sombor index	$\sum_{wv\in\mathcal{E}(\mathcal{G})} \sqrt{(d_w(\mathcal{G}))^2 + (d_v(\mathcal{G}))^2}$	[32]

Table 2.2: Topological indices w.r.t. degrees

2.2 Analysis of Sombor index

In this section, we introduce Sombor index and its variants.

Sombor index

A well known and widely used degree of vertex based topological index is Sombor index, introduced and studied by Gutman [32]. It has been applied in various fields, including chemistry, bioinformatics, and network analysis. Sombor index of a graph $\mathcal{G}$ in [32, 46] is defined as

$$\mathcal{SO}(\mathcal{G}) = \sum_{uv \in \mathcal{E}(\mathcal{G})} \sqrt{(d_u(\mathcal{G}))^2 + (d_v(\mathcal{G}))^2}. \tag{2.1}$$

The sum encompasses all edges within $\mathcal{G}$. The expression $\sqrt{(d_u(\mathcal{G}))^2 + ((\mathcal{G}))^2}$ demonstrates the degree radius of the edge uv in $\mathcal{G}$. This degree radius represents the distance between the ordered pair $(d_u(\mathcal{G}), d_v(\mathcal{G}))$ and the origin $(0, 0)$, $d_u(\mathcal{G}) \leq d_v(\mathcal{G})$.

Reduced Sombor index

The reduced Sombor index denoted by $\mathcal{SO}_{red}(\mathcal{G})$ refers to the distance in between the degree point of any edge in a graph $\mathcal{G}$ and the degree point of an isolated edge, which is defined as $(1, 1)$. It can be defined as

$$\mathcal{SO}_{red}(\mathcal{G}) = \sum_{uv \in \mathcal{E}(\mathcal{G})} \sqrt{(d_u(\mathcal{G}) - 1)^2 + (d_v(\mathcal{G}) - 1)^2}.$$

Average Sombor index

The average Sombor index, represented by $SO_{avg}(\mathcal{G})$ is the distance in between degree points of a graph $\mathcal{G}$ and the average degree point $(\frac{2m(\mathcal{G})}{n(\mathcal{G})}, \frac{2m(\mathcal{G})}{n(\mathcal{G})})$, is calculated as follows

$$\mathcal{SO}_{avg}(\mathcal{G}) = \sum_{uv \in \mathcal{E}(\mathcal{G})} \sqrt{\left(d_u(\mathcal{G}) - \frac{2m(\mathcal{G})}{n(\mathcal{G})}\right)^2 + \left(d_v(\mathcal{G}) - \frac{2m(\mathcal{G})}{n(\mathcal{G})}\right)^2}.$$

Sombor indices of some special graphs

Sombor indices of some special graphs of order n can be seen in Table 2.3.

Names of graphs	Sombor index
Complete graph	$SO(K_n) = \frac{n(n-1)^2}{\sqrt{2}}$
Complement of complete graph	$SO(K'_n) = 0$
Cycle graph	$SO(C_n) = 2\sqrt{2}n$
Star graph	$SO(S_n) = (n-1)\sqrt{n^2-2n+2}$
Bipartite graph when n is even	$SO(\mathcal{G}) \leq \frac{n^3}{\sqrt{32}}$
Bipartite graph when n is odd	$SO(\mathcal{G}) \leq \frac{n^2\sqrt{n^2+1}-\sqrt{n^2+1}}{\sqrt{32}}$
Path $n \geq 3$	$SO(P_n) = 2\sqrt{5} + 2(n-3)\sqrt{2}$

Table 2.3: Sombor index of some special graphs

2.2.1 Some basic results of Sombor index

In this section, we give some known results about Sombor index.

Theorem 2.2.1. [43] *Let $\mathcal{G}$ be a graph with size m and smallest degree δ. Then*

$$\mathcal{SO}(\mathcal{G}) \leq \mathcal{Z}_1(\mathcal{G}) + (\sqrt{2}-2)\delta m,$$

where $\mathcal{Z}_1(\mathcal{G})$ is the first Zagreb index of graph $\mathcal{G}$. Furthermore, the equality holds if and only if $\mathcal{G}$ is a regular graph.

Theorem 2.2.2. [43] *Let $\mathcal{G}$ be a graph with n vertices and m edges. The maximum degree is represented as Δ , while its smallest degree is $\delta > 0$. Then*

$$\mathcal{SO}(\mathcal{G}) \geq \frac{\sqrt{\Delta^2+\delta^2}\mathcal{Z}_1(\mathcal{G}) + \sqrt{2}\Delta\delta m + \sqrt{2}\delta\delta m}{\sqrt{2}\sqrt{(\Delta^2+\delta^2)} + \Delta + \delta},$$

The equality holds if and only if $\mathcal{G}$ is a regular graph.

Theorem 2.2.3. [43] *Let $\mathcal{G}$ be a graph with m edges. Assuming that $\mathcal{G}$ has a maximum degree of Δ and a smallest degree $\delta > 0$. Then*

$$\mathcal{SO}(\mathcal{G}) \leq \left[\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right] m\mathcal{Z}_2(\mathcal{G}),$$

where $\mathcal{Z}_2(\mathcal{G})$ is the second Zagreb index of graph $\mathcal{G}$. Furthermore, the equality occurs if and only if $\mathcal{G}$ is a regular graph or a bipartite semi-regular graph.

Theorem 2.2.4. [43] *Let $\mathcal{G}$ be a graph with n vertices. Assuming that $\mathcal{G}$ has a maximum degree of Δ and smallest degree $\delta > 0$. Then*

$$\mathcal{SO}(\mathcal{G}) \geq \frac{2Z_2(\mathcal{G}) + n\Delta\delta^2}{\sqrt{2}(\Delta + \delta)},$$

The equality occurs if and only if $\mathcal{G}$ is a regular graph or a bipartite semi-regular graph.

Theorem 2.2.5. [44] *Consider a graph $\mathcal{G}$ of size m. Then*

$$\mathcal{SO}(\mathcal{G}).\mathcal{R}(\mathcal{G}) \geq \sqrt{2}m^2,$$

where $\mathcal{R}(\mathcal{G})$ is Randić index of graph $\mathcal{G}$ and equality occurs if and only if $\mathcal{G}$ is regular.

Theorem 2.2.6. [45] *Assume that $\mathcal{G}$ is a chemical graph of order n. Then,*

$$\mathcal{SO}(\mathcal{G}) = 8\sqrt{2}n,$$

equality holds if and only if $\mathcal{G}$ is 4-regular graph.

Theorem 2.2.7. [45] *Assume that $\mathcal{G}$ is a chemical tree of order n. Then,*

$$8\sqrt{2}v \geq \mathcal{SO}(\mathcal{G}) \geq 2\sqrt{5} + 2\sqrt{2}(n-3).$$

The right inequality changes into equality if and only if $\mathcal{G}$ is isomorphic to a $\mathcal{P}_n$ graph. The left inequality changes into equality if and only if $\mathcal{G}$ is isomorphic to a 4-regular graph.

Theorem 2.2.8. [45] *Assume that $\mathcal{C}_n$ is a chemical tree of order $n \geq 3$. Then,*

$$\mathcal{SO}(\mathcal{G}) \leq \frac{2\sqrt{17} + 4\sqrt{2}}{3}n - \frac{20\sqrt{2} - 2\sqrt{17}}{3}.$$

Equality occurs if and only if $\mathcal{C}_n$ does not have a vertex of degree 2 and 3.

Theorem 2.2.9. [45] *Assume that $\mathcal{C}_n$ be chemical trees with n vertices, consider the following subsets of $\mathcal{C}_n$,*

$\mathcal{C}_{00} = \{\mathcal{T} \in \mathcal{C}_n : d_G(v_2) = d_G(v_3) = 0\}$

$\mathcal{C}_{10} = \{\mathcal{T} \in \mathcal{C}_n : d_G(v_2) = 1, d_G(v_3) = 0\}$

$\mathcal{C}_{01} = \{\mathcal{T} \in \mathcal{C}_n : d_G(v_2) = 0, d_G(v_3) = 1\}.$

Then, maximum value of Sombor index amoung all chemical trees of order n is attained in:

(i) $\mathcal{T} \in \mathcal{C}_{00}(n)$ *if* $n \equiv 2 (\mathrm{mod}\, 3)$ *for* $n \geq 5$.

(ii) $\mathcal{T} \in \mathcal{C}_{10}(n)$ *with* $m_{1,2} = 0$ *if* $n \equiv 0 (\mathrm{mod}\, 3)$ *for* $n \geq 9$.

(iii) $\mathcal{T} \in \mathcal{C}_{01}(n)$ *with* $m_{1,3} = 0$ *if* $n \equiv 1 (\mathrm{mod}\, 3)$ *for* $n \geq 13$.

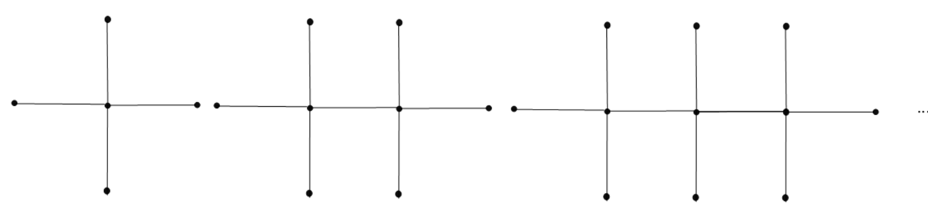

Figure 2.1: Trees in C_{00}

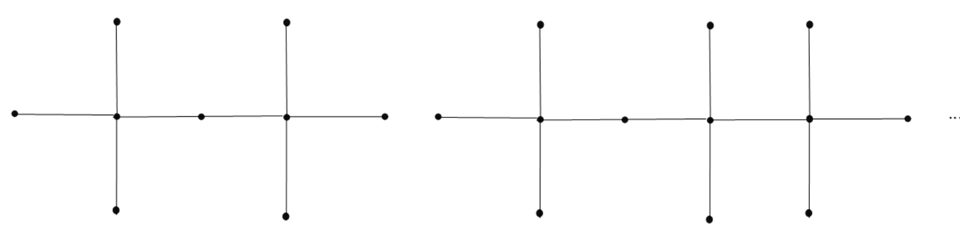

Figure 2.2: Trees in C_{10}

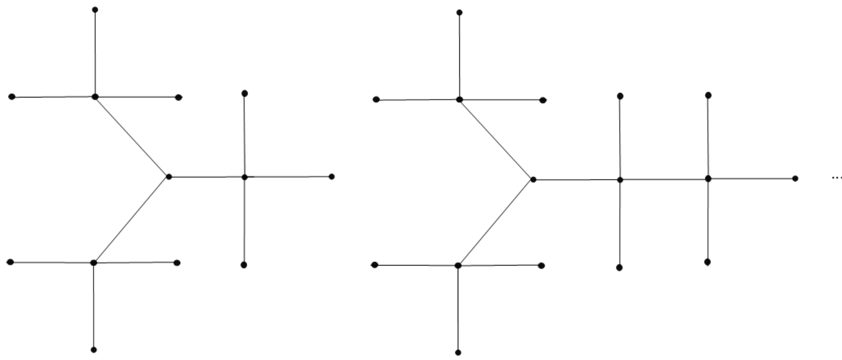

Figure 2.3: Trees in C_{01}

Monotonic functions and extermal Sombor index

Lemma 2.2.1. *Let* $f(x) = \sqrt{(s-t)^2 + x^2} - \sqrt{s^2 + x^2}$, *where* $s > t > 0$ *and* $x > 0$ *are real numbers. Then* $f(x)$ *is a strictly increasing function.*

Proof.

$$\frac{df(x)}{dx} = \frac{x}{\sqrt{x^2 + (s-t)^2}} - \frac{x}{\sqrt{x^2 + s^2}} > 0.$$

Thus $f(x)$ is a strictly increasing function. □

Lemma 2.2.2. *Let* $f(x) = \sqrt{s^2 + x^2} - \sqrt{(s-t)^2 + x^2}$, *where* $s > t > 0$ *and* $x > 0$ *are real numbers. Then* $f(x)$ *is a strictly decreasing function.*

Proof.

$$\frac{df(x)}{dx} = \frac{x}{\sqrt{x^2 + s^2}} - \frac{x}{\sqrt{x^2 + (s-t)^2}} < 0.$$

Thus $f(x)$ is a strictly decreasing function. □

Chapter 3

Maximum Sombor index of chemical trees with given vertices of maximum degree

In the field of chemical graph theory, the study of topological indices mainly deals with addressing significant and extensively researched problems. These studies focus on the identification of chemical structures that attain the maximum or minimum values of specific topological indices while adhering to predefined criteria. Assume that $\mathcal{C}(n, k)$ be a class of chemical trees of order n and fixed vertex k of degree 4 for $k \geq 1$. In this chapter, we focus on determining the maximum Sombor index values of $\mathcal{C}(n, k)$.

3.1 Preliminaries

In this section, we provide some lemmas and terminologies of chemical graph theory that are required in sequel. Let

$$A = \{(u, v) \in \mathbb{N} \times \mathbb{N} \backslash (1, 1) : 1 \leq u \leq v \leq 4\},$$

where $\mathbb{N}$ is the set of natural numbers. Sombor index for chemical trees can also be expressed as

$$SO(T) = \sum_{(u,v) \in A} \sqrt{u^2 + v^2} \quad m_{u,v}. \tag{3.1}$$

In [45], following relations are given:

$$n_1 + n_2 + n_3 + n_4 = n, \tag{3.2a}$$

$$n_1 + 2(n_2) + 3(n_3) + 4(n_4) = 2(n-1), \tag{3.2b}$$

$$2(m_{1,1}) + m_{1,2} + m_{1,3} + m_{1,4} = n_1, \tag{3.2c}$$

$$m_{1,2} + 2(m_{2,2}) + m_{2,3} + m_{2,4} = 2n_2, \tag{3.2d}$$

$$m_{1,3} + m_{2,3} + 2(m_{3,3}) + m_{3,4} = 3n_3, \tag{3.2e}$$

$$m_{1,4} + m_{2,4} + m_{3,4} + 2(m_{4,4}) = 4n_4. \tag{3.2f}$$

Lemma 3.1.1. *Assume that a tree $T \in \mathcal{C}(n,k)$ has maximum Sombor index. Then $n_2 \leq 1$.*

Proof. On contrary, assume that $n_2 > 1$. Let $\{u, v\} \in V(T)$ such that $d_T(u) = d_T(v) = 2$. We consider two cases:

Case 1. When $uv \in E(T)$. Let $u_1 \in N_T(u)\backslash\{v\}$ and $v_1 \in N_T(v)\backslash\{u\}$. Let T^* be another tree obtained from T, as follows:

$$T^* = T - uu_1 + vu_1.$$

Then $T^* \in \mathcal{C}(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in \{V(T)\backslash\{u,v\}\}$ where $d_T(v)+1 = d_{T^*}(v)$ and $d_T(u) - 1 = d_{T^*}(u)$. Then we get

$$\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(u_1) + (d_T(v)+1)^2} + \sqrt{(d_T(u)-1)^2 + (d_T(v)+1)^2} \\
&+ \sqrt{(d_T(v)+1)^2 + d_T^2(v_1)} - \sqrt{d_T^2(u_1) + d_T^2(u)} - \sqrt{d_T^2(u) + d_T^2(v)} \\
&- \sqrt{d_T^2(v) + d_T^2(v_1)} \\
&= \sqrt{d_T^2(u_1) + (2+1)^2} + \sqrt{(2-1)^2 + (2+1)^2} \\
&+ \sqrt{(2+1)^2 + d_T^2(v_1)} - \sqrt{d_T^2(u_1) + 2^2} - \sqrt{2^2 + 2^2} \\
&- \sqrt{2^2 + d_T^2(v_1)}
\end{aligned}$$

$$
\begin{aligned}
&= \sqrt{d_T^2(u_1)+9} + \sqrt{1+9} + \sqrt{9+d_T^2(v_1)} - \sqrt{d_T^2(u_1)+4} \\
&- \sqrt{4+4} - \sqrt{4+d_T^2(v_1)} \\
&= \sqrt{16+9} + \sqrt{10} + \sqrt{9+16} - \sqrt{16+4} - \sqrt{8} - \sqrt{4+16} \\
&= 1.3895 > 0.
\end{aligned}
$$

By using Lemma 2.2.1, we obtain $SO(T^*) - SO(T) > 0$, which is a contradiction since T has maximum Sombor index. Hence, there cannot be adjacent vertices of degree 2 in T.

Case 2. When $uv \notin E(T)$. Let $\{u_1, u_2\} \in N_T(u)$ and $\{v_1, v_2\} \in N_T(v)$. Without loss of generality, assume that there exists a $u, v-$path where u_1 and v_1 are lying on it. Then it is clear that $d_T(u_1) \geq 2$ and $d_T(v_1) \geq 2$.

Subcase 1. When at most 1 vertex in $\{u_1, u_2, v_1, v_2\}$ has degree 4. Without loss of generality, assume $d_T(u_2) = 4$. Let T^* be another tree obtained from T, as follows:

$$T^* = T - uu_2 + vu_2.$$

Then $T^* \in \mathcal{C}(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in \{V(T) \backslash \{v, u\}\}$ where $d_{T^*}(u) = d_T(u) - 1$ and $d_{T^*}(v) = d_T(v) + 1$. Then we get

$$
\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(u_2) + (d_T(v)+1)^2} + \sqrt{d_T^2(v_1) + (d_T(v)+1)^2} \\
&+ \sqrt{(d_T(v_2)^2 + (d_T(v)+1)^2} + \sqrt{(d_T(u)-1)^2 + d_T^2(u_1)} \\
&- \sqrt{d_T^2(u_2) + d_T^2(u)} - \sqrt{d_T^2(v_1) + d_T^2(v)} - \sqrt{d_T^2(v_2) + d_T^2(v)} \\
&- \sqrt{d_T^2(u) + d_T^2(u_1)} \\
&= \sqrt{d_T^2(u_2) + 3^2} + \sqrt{d_T^2(v_1) + 3^2} + \sqrt{d_T^2(v_2) + 3^2} + \sqrt{1^2 + d_T^2(u_1)} \\
&- \sqrt{d_T^2(u_2) + 2^2} - \sqrt{d_T^2(v_1) + 2^2} - \sqrt{d_T^2(v_2) + 2^2} - \sqrt{2^2 + d_T^2(u_1)} \\
&= \sqrt{4^2+3^2} + \sqrt{3^2+3^2} + \sqrt{3^2+3^2} + \sqrt{1^2+2^2} - \sqrt{4^2+2^2} \\
&- \sqrt{3^2+2^2} - \sqrt{3^2+2^2} - \sqrt{2^2+2^2} \\
&= 1.20 > 0.
\end{aligned}
$$

By using Lemmas 2.2.1 and 2.2.2, we obtain $SO(T^*) - SO(T) > 0$, which is a contradiction since T has maximum Sombor index.

Subcase 2. When at least two vertices in $\{u_1, u_2, v_1, v_2\}$ have degree 4. Without loss of generality, assume $d_T(u_1) = d_T(u_2) = 4$. Let T^* be another tree obtained from T, as follows:

$$T^* = T - uu_1 - uu_2 + u_1u_2 + vu.$$

Then $T^* \in \mathcal{C}(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in \{V(T)\backslash\{v,u\}\}$ where $d_{T^*}(u) = d_T(u) - 1$ and $d_{T^*}(v) = d_T(v) + 1$. Then we get

$$\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(u_1) + d_T^2(u_2)} + \sqrt{d_T^2(v_1) + (d_T(v)+1)^2} \\
&+ \sqrt{(d_T(v)+1)^2 + (d_T(u)-1)^2} + \sqrt{(d_T(v)+1)^2 + d_T^2(v_2)} \\
&- \sqrt{d_T^2(u_1) + d_T^2(u)} - \sqrt{d_T^2(u) + d_T^2(u_2)} - \sqrt{d_T^2(v) + d_T^2(v_1)} \\
&- \sqrt{d_T^2(v) + d_T^2(v_2)} \\
&= \sqrt{d_T^2(u_1) + d_T^2(u_2)} + \sqrt{d_T^2(v_1) + 3^2} + \sqrt{3^2 + 1^2} + \sqrt{3^2 + d_T^2(v_2)} \\
&- \sqrt{d_T^2(u_1) + 2^2} - \sqrt{2^2 + d_T^2(u_2)} - \sqrt{2^2 + d_T^2(v_1)} - \sqrt{2^2 + d_T^2(v_2)} \\
&= \sqrt{4^2 + 4^2} + \sqrt{4^2 + 3^2} + \sqrt{3^2 + 1^2} + \sqrt{3^2 + 4^2} \\
&- \sqrt{4^2 + 2^2} - \sqrt{2^2 + 4^2} - \sqrt{2^2 + 4^2} - \sqrt{2^2 + 4^2} \\
&= 0.930 > 0.
\end{aligned}$$

Using Lemma 2.2.2, we obtain $SO(T^*) - SO(T) > 0$, which is a contradiction since T has maximum Sombor index. Thus $n_2 \leq 1$. This finishes the proof. $\square$

Lemma 3.1.2. *Assume that a tree $T \in \mathcal{C}(n,k)$ has maximum Sombor index and $n-k$ is even. Then*

(i) $n_2 = 0$

(ii) $n_1 = \frac{n}{2} + \frac{k}{2} + 1$, $n_3 = \frac{n}{2} - \frac{3k}{2} - 1$.

Proof.

(i) Since $n-k$ is even, that is, $n-k=2l$, for some positive integer l. On contrary, assume that $n_2 \geq 1$. By Lemma 3.1.1, $n_2 \leq 1$. Thus $n_2 = 1$. We consider two cases:

Case 1. When both n and $k = n_4$ are even, that is, $n = 2l_1$ and $n_4 = 2l_2$ for some positive integers l_1 and l_2. Substituting n, n_2 and n_4 in Equation (3.2a) we obtain

$$2l_1 = n_1 + 1 + n_3 + 2l_2. \tag{3.3}$$

Using Lemma 1.3.1, we know that $n_1 + n_3 = 2l_3$ for some positive integer l_3. Now Equation (3.3) becomes

$$2l_1 \neq 2l_3 + 2l_2 + 1, \tag{3.4}$$

Equation (3.4) contradicts Equation (3.3). Hence $n_2 = 0$.

Case 2. When both n and $k = n_4$ are odd, that is, $n = 2l_1 - 1$ and $n_4 = 2l_2 - 2$ for some positive integers l_1 and l_2. Substituting n, n_2 and n_4 in Equation (3.2a) we obtain

$$2l_1 - 1 = n_1 + 1 + n_3 + 2l_2 - 1.$$

By using the same argument as in Case 1, we can conclude that $n_2 = 0$.

(ii) By Part (i), $n_2 = 0$. Thus Equations (3.2a) and (3.2b) become

$$n = n_1 + n_3 + k \tag{3.5}$$

$$2n - 2 = n_1 + 3n_3 + 4k. \tag{3.6}$$

Simultaneously solving Equations (3.5) and (3.6), we obtain

$$n_1 = \frac{n}{2} + \frac{k}{2} + 1,$$

$$n_3 = \frac{n}{2} - \frac{3k}{2} - 1.$$

This finishes the proof. $\square$

Lemma 3.1.3. *Assume that a tree $T \in \mathcal{C}(n,k)$ has maximum Sombor index and $n-k$ is odd. Then*

(i) $n_2 = 1$

(ii) $n_1 = \frac{n+k+1}{2}$, $n_3 = \frac{n-3k-3}{2}$.

Proof.

(i) Since $n-k$ is odd, that is, $n-k = 2l-1$, for some integer l. By Lemma 3.1.1, $n_2 \leq 1$. On contrary, we assume that $n_2 = 0$. We consider two cases:

Case 1. When n is even and $k = n_4$ is odd, that is, $n = 2l_1$ and $n_4 = 2l_2 - 1$ for some positive integers l_1 and l_2. Substituting n, n_2 and n_4 in Equation (3.2a), we obtain

$$2l_1 = n_1 + 0 + n_3 + 2l_2 - 1. \tag{3.7}$$

Using Lemma 1.3.1, we know that $n_1 + n_3 = 2l_3$ for some integer l_3. Now Equation (3.6) becomes

$$2l_1 \neq 2l_3 + 2l_2 - 1, \tag{3.8}$$

Equation (3.8) contradicts Equation (3.7). Hence $n_2 = 1$.

Case 2. When n is odd and $k = n_4$ is even, that is, $n = 2l_1 - 1$ and $n_4 = 2l_2$ for some positive integers l_1 and l_2. Substituting n, n_2 and n_4 in (3.2a) we obtain

$$2l_1 - 1 = n_1 + 0 + n_3 + 2l_2$$

By using the same argument as in Case 1, we can conclude that $n_2 = 1$.

(ii) By Part (i), $n_2 = 1$. Thus Equations (3.2a) and (3.2b) become

$$n = n_1 + 1 + n_3 + k \tag{3.9}$$

$$2n - 2 = n_1 + 2 + 3n_3 + 4k. \tag{3.10}$$

Simultaneously solving Equations (3.9) and (3.10), we obtain

$$n_1 = \frac{n+k+1}{2},$$

$$n_3 = \frac{n-3k-3}{2}.$$

This completes the proof. $\square$

Consider the following subsets of $\mathcal{C}(n,k)$:

$$C_1(n,k) = \{T \in \mathcal{C}(n,k) : 3k+3 \leq n \leq 4k, k \geq 3\}, \tag{3.11a}$$

$$\mathcal{C}_2(n,k) = \{T \in \mathcal{C}(n,k) : 4k < n < 5k-2, k \geq 4\} \cup \{T \in \mathcal{C}(n,k) : n = 9, k = 2\}, \tag{3.11b}$$

$$\mathcal{C}_3(n,k) = \{T \in \mathcal{C}(n,k) : n \geq 5k-2, k \geq 3\} \cup \{T \in \mathcal{C}(n,k) : n \geq 3k+4, k \in \{1,2\}\}. \tag{3.11c}$$

Lemma 3.1.4. *Assume that a tree $T \in \mathcal{C}_1(n,k)$ has maximum Sombor index and $n-k$ is even. Then*

(i) $m_{4,4} \neq 0$

(ii) $m_{2,2} = m_{1,2} = m_{2,3} = m_{2,4} = 0$

(iii) $m_{1,3} = m_{3,3} = 0$

(iv) $m_{3,4} = \frac{3n}{2} - \frac{9k}{2} - 3$, $m_{1,4} = \frac{n}{2} + \frac{k}{2} + 1$, $m_{4,4} = 4k - n + 1$.

Proof.

(i) On contrary, assume that $m_{4,4} = 0$. From Equation (3.2f), we get

$$m_{1,4} + m_{2,4} + m_{3,4} = 4k. \tag{3.12}$$

It is obvious by Equation (3.2c) that $m_{1,4} \leq n_1$. Also, by Lemma 3.1.2 (i), $n_2 = 0$. Then Equation (3.12) becomes

$$m_{3,4} = 4k - m_{1,4},$$

$$m_{3,4} \geq 4k - n_1. \tag{3.13}$$

From Lemma 3.1.2 (ii), we know that $n_1 = \frac{n}{2} + \frac{k}{2} + 1$. By Equation (3.11a), we have $n \leq 4k$. Now Equation (3.12) becomes

$$m_{3,4} \geq 4k - (\tfrac{n}{2} + \tfrac{k}{2} + 1),$$

$$m_{3,4} \geq \tfrac{3k}{2} - 1. \tag{3.14}$$

Also we know by Equation (3.2e) that $m_{3,4} \leq 3n_3$. Now substituting $n_3 = \frac{n}{2} - \frac{3k}{2} - 1$ from Lemma 3.1.2 (ii), we get

$$m_{3,4} \leq \tfrac{3k}{2} - 3. \tag{3.15}$$

Equation (3.15) contradicts Equation (3.14). Hence, $m_{4,4} \neq 0$.

(ii) This result is a direct consequence of Lemma 3.1.2 (i).

(iii) On contrary, we assume that $m_{1,3} \neq 0$ (or $m_{3,3} \neq 0$) that is, $uv \in E(T)$ such that $d_T(u) = 1$ (or $d_T(u) = 3$) and $d_T(v) = 3$. Let $\{v_1, v_2\} = N_T(v) \backslash \{u\}$. By (i) we know that there is an edge $xy \in E(T)$ such that $d_T(x) = d_T(y) = 4$. Without loss of generality, assume $vx-$path containing vv_1. Now, Let T^* be another tree obtained from T, as follows:

$$T^* = T - uv - vv_1 - xy + uv_1 + xv + vy.$$

Then $T^* \in \mathcal{C}_1(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)$. Then we get

$$\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(x) + d_T^2(v)} + \sqrt{d_T^2(v) + d_T^2(y)} + \sqrt{d_T^2(u) + d_T^2(v_1)} \\
&- \sqrt{d_T^2(u) + d_T^2(v)} - \sqrt{d_T^2(x) + d_T^2(y)} - \sqrt{d_T^2(v) + d_T^2(v_1)} \\
&= \sqrt{4^2 + 3^2} + \sqrt{3^2 + 4^2} + \sqrt{1^2 + d_T^2(v_1)} - \sqrt{1^2 + 3^2} - \sqrt{4^2 + 4^2} \\
&- \sqrt{3^2 + d_T^2(v_1)} \\
&= \sqrt{4^2 + 3^2} + \sqrt{3^2 + 4^2} + \sqrt{1^2 + 3^2} - \sqrt{1^2 + 3^2} - \sqrt{4^2 + 4^2} \\
&- \sqrt{3^2 + 3^2} \\
&= 0.10 > 0.
\end{aligned}$$

By using Lemma 2.2.1, we obtain $SO(T^*) - SO(T) > 0$, which is a contradiction since T has maximum Sombor index. Hence, $m_{1,3} = 0$ (or $m_{3,3} = 0$).

(iv) Using the values of n_1, n_2 and n_3 from Lemma 3.1.2 and the values of edges obtained from (i) to (iii) in Equations (3.2c),(3.2e) and (3.2f), we obtain

$$\begin{aligned} m_{1,4} &= \frac{n}{2} + \frac{k}{2} + 1, \\ m_{3,4} &= \frac{3n}{2} - \frac{9k}{2} - 3, \\ m_{4,4} &= 4k - n + 1. \end{aligned}$$

This finishes the proof. □

Lemma 3.1.5. *Assume that a tree $T \in \mathcal{C}_1(n,k)$ has maximum Sombor index and $n-k$ is odd. Then*

(i) $m_{4,4} \neq 0$

(ii) $m_{2,2} = m_{1,2} = 0$

(iii) $m_{2,3} = m_{1,3} = m_{3,3} = 0$

(iv) $m_{3,4} = \frac{3n-9k-9}{2}$, $m_{1,4} = \frac{n+k+1}{2}$, $m_{2,4} = 2$, $m_{4,4} = 4k - n + 1$.

Proof.

(i) On contrary, assume that $m_{4,4} = 0$. Using in Equation (3.2e), we get

$$m_{1,4} + m_{2,4} + m_{3,4} = 4k. \tag{3.16}$$

Clearly by Equation (3.2c) we have $m_{1,4} \leq n_1$. By Lemma 3.1.3 (i), $m_{2,4} \leq 2$ and by Lemma 3.1.3 (ii), $n_1 = \frac{n+k+1}{2}$. By Equation (3.11a) we have $n \leq 4k$. This implies

$$\begin{aligned} m_{3,4} &= 4k - m_{1,4} - m_{2,4} \\ &\geq 4k - \frac{n+k+1}{2} - 2 \\ &\geq 4k - \frac{4k+k+1}{2} - 2 \end{aligned}$$

$$m_{3,4} \geq \tfrac{3k-5}{2}. \tag{3.17}$$

Also we know by Equation (3.2e) that $m_{3,4} \leq 3n_3$. Now by Lemma 3.1.3(ii) we know that $n_3 = \frac{n-3k-3}{2}$, we get

$$m_{3,4} \leq \frac{3k-9}{2}. \tag{3.18}$$

Equation (3.18) contradicts Equation (3.17). Hence, $m_{4,4} \neq 0$.

(ii) Proof of $m_{2,2} = 0$ is the direct consequence of Lemma 3.1.3 (i). Now on contrary, assume that $m_{1,2} \neq 0$, that is, there exists an edge $uv \in E(T)$ such that $d_T(u) = 1$ and $d_T(v) = 2$. Let $N_T(v)\backslash\{u\} = \{v_1\}$. By (i), there is an edge $xy \in E(T)$ such that $d_T(x) = d_T(y) = 4$. Without loss of generality assume that there exist $u, x-$path containing y. Let T^* be another tree obtained from T, as follows:

$$T^* = T - uv - vv_1 - xy + uv_1 + xv + vy.$$

Then $T^* \in \mathcal{C}_1(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)$. Then we get

$$\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(x) + d_T^2(v)} + \sqrt{d_T^2(v) + d_T^2(y)} + \sqrt{d_T^2(u) + d_T^2(v_1)} \\
&\quad - \sqrt{d_T^2(u) + d_T^2(v)} - \sqrt{d_T^2(x) + d_T^2(y)} - \sqrt{d_T^2(v) + d_T^2(v_1)} \\
&= \sqrt{4^2 + 2^2} + \sqrt{2^2 + 4^2} + \sqrt{1^2 + d_T^2(v_1)} - \sqrt{1^2 + 2^2} - \sqrt{4^2 + 4^2} \\
&\quad - \sqrt{2^2 + d_T^2(v_1)} \\
&= \sqrt{4^2 + 2^2} + \sqrt{2^2 + 4^2} + \sqrt{1^2 + 3^2} - \sqrt{1^2 + 2^2} - \sqrt{4^2 + 4^2} \\
&\quad - \sqrt{2^2 + 3^2} \\
&= 0.60 > 0.
\end{aligned}$$

By using Lemma 2.2.1, we obtain $SO(T^*) - SO(T) > 0$, which is a contradiction since T has maximum Sombor index. Hence, $m_{1,2} = 0$.

(iii) On contrary, assume that $m_{2,3} \neq 0$. Then there exists an edge $uv \in E(T)$ such that $d_T(u) = 3$ and $d_T(v) = 2$. Let $N_T(v)\backslash\{u\} = \{v_1\}$. By (i) we know that an edge

$xy \in E(T)$ such that $d_T(x) = d_T(y) = 4$. Without loss of generality assume that there exist $v_1, x-$path containing y. Let T^* be another tree obtained from T, as follows:

$$T^* = T - uv - vv_1 - xy + uv_1 + xv + vy.$$

Then $T^* \in \mathcal{C}_1(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)$. Then we get

$$\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(x) + d_T^2(v)} + \sqrt{d_T^2(v) + d_T^2(y)} + \sqrt{d_T^2(u) + d_T^2(v_1)} \\
&-\sqrt{d_T^2(u) + d_T^2(v)} - \sqrt{d_T^2(x) + d_T^2(y)} - \sqrt{d_T^2(v) + d_T^2(v_1)} \\
&= \sqrt{4^2 + 2^2} + \sqrt{2^2 + 4^2} + \sqrt{3^2 + d_T^2(v_1)} - \sqrt{3^2 + 2^2} - \sqrt{4^2 + 4^2} \\
&-\sqrt{2^2 + d_T^2(v_1)} \\
&= \sqrt{4^2 + 2^2} + \sqrt{2^2 + 4^2} + \sqrt{3^2 + 4^2} - \sqrt{3^2 + 2^2} - \sqrt{4^2 + 4^2} \\
&-\sqrt{2^2 + 4^2} \\
&= 0.20 > 0.
\end{aligned}$$

By using Lemma 2.2.2, we obtain $SO(T^*) - SO(T) > 0$, which is a contradiction since T has maximum Sombor index. Hence, $m_{2,3} = 0$.

Proofs of $m_{1,3} = 0$ and $m_{3,3} = 0$ are similar to Lemma 3.1.4(iii).

(iv) By putting the values of n_1, n_2 and n_3 from Lemma 3.1.3 and values of edges obtained from (i) to (iii) in Equations (3.2c) to (3.2f) we obtain

$$\begin{aligned}
m_{1,4} \quad &= \frac{n+k+1}{2}, \\
m_{2,4} \quad &= 2, \\
m_{3,4} \quad &= \frac{3n-9k-9}{2}, \\
m_{4,4} \quad &= 4k - n + 1.
\end{aligned}$$

This completes the proof. □

Lemma 3.1.6. *Assume that a tree $T \in \mathcal{C}_2(n,k)$ has maximum Sombor index and $n-k$ is even. Then*

(i) $m_{2,2} = m_{1,2} = m_{2,3} = m_{2,4} = 0$

(ii) $m_{4,4} = 0$

(iii) $m_{1,3} = 0$

(iv) $m_{3,4} = \frac{7k}{2} - \frac{n}{2} - 1$, $m_{1,4} = \frac{n}{2} + \frac{k}{2} + 1$, $m_{3,3} = n - 4k - 1$.

Proof.

(i) This result is a direct outcome of Lemma 3.1.2 (i).

(ii) On contrary, assume that $m_{4,4} \neq 0$, that is, there exists an edge $xy \in E(T)$ with $d_T(x) = d_T(y) = 4$. First we claim that $m_{1,3} \neq 0$ and $m_{3,3} \neq 0$. To prove this, on contrary assume that $m_{1,3} = 0$ and $m_{3,3} = 0$. Using (i) in Equations (3.2c) and (3.2f) imply,

$$m_{1,4} = n_1, \tag{3.19}$$

$$m_{3,4} = 3n_3. \tag{3.20}$$

Using Equations (3.19) and (3.20) in (3.2f) we obtain $2m_{4,4} = 4k - n_1 - 3n_3$. By substituting the values of n_1 and n_3 from Lemma 3.1.2 we have $m_{4,4} = 4k - n + 1$ further implies that $m_{4,4} \leq 0$. Using Equation (3.11b), we have $n \geq 4k + 1$ which is a contradiction. Now, we discuss two cases.

Case 1. If $m_{1,3} \neq 0$ then $m_{4,4} = 0$.
Proof is similar to Lemma 3.1.4 (iii).

Case 2. If $m_{3,3} \neq 0$ then $m_{4,4} = 0$.
Proof is similar to Lemma 3.1.4 (iv).

(iii) On contrary, assume that $m_{1,3} \neq 0$, then there exists an edge $xy \in E(T)$ such that $d_T(x) = 1$ and $d_T(y) = 3$. This indicates that $m_{1,4} < n_1$. Now by using value of n_1 from Lemma 3.1.2 (ii), we get $m_{1,4} < \frac{n}{2} + \frac{k}{2} + 1$. Using Equation (3.11b), we get $m_{1,4} < \frac{5k-2}{2} + \frac{k}{2} + 1 = 3k$. This implies that there exists a vertex u with degree $d_T(u) = 4$ with at most 2 pendent vertices. Let $\{u_1, u_2, s, t\} \in N_T(u)$ and $\{y_1, y_2\} \in N_T(y) \setminus \{x\}$ where $d_T(u_1) \neq 1$ and $d_T(u_2) \neq 1$. Without loss of generality, assume that there exist a $yu-$path containing yy_1 and u_1u. Now $d_T(u_2) = 3$ as by (i) and (ii) we have $m_{2,4} = 0$ and $m_{4,4} = 0$, respectively. Let T^* be another tree obtained from T, as follows:

$$T^* = T - u_2s - u_2t + xw + xz.$$

Then $T^* \in \mathcal{C}_2(n,k)$. Clearly $d_{T^*}(z) = d_T(z)$ for all $z \in \{V(T)\backslash\{u_2, x\}\}$ where $d_{T^*}(u_2) = d_T(u_2) - 2$ and $d_{T^*}(x) = d_T(x) + 2$. Then we get

$$\begin{aligned}
SO(T^*) - SO(T) \quad & = \sqrt{d_T^2(s) + (d_T(x)+2)^2} + \sqrt{d_T^2(t) + (d_T(x)+2)^2} \\
& + \sqrt{(d_T(x)+2)^2 + d_T^2(y)} + \sqrt{d_T^2(u) + (d_T(u_2)-2)^2} \\
& - \sqrt{d_T^2(u) + d_T^2(u_2)} - \sqrt{d_T^2(u_2) + d_T^2(s)} \\
& - \sqrt{d_T^2(u_2) + d_T^2(t)} - \sqrt{d_T^2(x) + d_T^2(y)} \\
& = \sqrt{d_T^2(s) + 3^2} + \sqrt{d_T^2(t) + 3^2} + \sqrt{3^2 + 3^2} + \sqrt{4^2 + 1^2} \\
& - \sqrt{4^2 + 3^2} - \sqrt{3^2 + d_T^2(w)} - \sqrt{3^2 + d_T^2(z)} - \sqrt{1^2 + 3^2} \\
& = 0.20 > 0.
\end{aligned}$$

Here, we obtain $SO(T^*) - SO(T) > 0$, which is a contradiction since T has maximum Sombor index. Hence, $m_{1,3} = 0$.

(iv) By using the values of n_1 and n_3 from Lemma 3.1.2 (ii) and the values of edges obtained from (i) to (iii) in Equations (3.2c) to (3.2f), we obtain

$$\begin{aligned}
m_{3,4} \quad & = \frac{7k}{2} - \frac{n}{2} - 1, \\
m_{1,4} \quad & = \frac{n}{2} + \frac{k}{2} + 1, \\
m_{3,3} \quad & = n - 4k - 1.
\end{aligned}$$

This completes the proof. □

Lemma 3.1.7. *Assume that a tree $T \in \mathcal{C}_2(n,k)$ has maximum Sombor index and $n-k$ is odd. Then*

(i) $m_{2,2} = m_{1,2} = 0$

(ii) $m_{4,4} = 0$

(iii) $m_{1,3} = 0$

(iv) $m_{2,4} = 2$

(v) $m_{2,3} = 0$, $m_{3,4} = \frac{7k-n-5}{2}$, $m_{1,4} = \frac{n+k+1}{2}$, $m_{3,3} = n - 4k - 1$.

Proof.

(i) By Lemma 3.1.3 (i) it is given that $n_2 = 1$. It is obvious that $m_{2,2} = 0$. Next, on contrary assume that $m_{1,2} \neq 0$, that is, there exists an edge $xy \in E(T)$ such that $d_T(x) = 1$ and $d_T(y) = 2$. Let $y_1 \in N_T(y) \setminus \{x\}$ and $d_T(u) = 4$ where $\{u_1, u_2, u_3, u_4\} = N_T(u)$. Without loss of generality, assume that their exist a $uy-$path containing yy_1 and uu_4. Let T^* be another tree obtained from T, as follows:

$$T^* = T - uu_1 - uu_2 - uu_3 + xu_1 + xu_2 + xu_3.$$

Then $T^* \in \mathcal{C}_2(n, k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T) \setminus \{u, x\}$ where $d_{T^*}(u) = d_T(u) - 3$ and $d_{T^*}(x) = d_T(x) + 3$. Then we get

$$\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(u_1) + (d_T(x)+3)^2} + \sqrt{d_T^2(u_2) + (d_T(x) + 3^2)} \\
&+ \sqrt{d_T^2(u_3) + (d_T(x)+3)^2} + \sqrt{(d_T(x)+3)^2 + d_T^2(y)} \\
&+ \sqrt{d_T^2(u_4) + (d_T(u)-3)^2} - \sqrt{d_T^2(u) + d_T^2(u_4)} - \sqrt{d_T^2(u) + d_T^2(u_1)} \\
&- \sqrt{d_T^2(u) + d_T^2(u_2)} - \sqrt{d_T^2(u) + d_T^2(u_3)} - \sqrt{d_T^2(x) + d_T^2(y)} \\
&= \sqrt{d_T^2(u_1) + 4^2} + \sqrt{d_T^2(u_2) + 4^2} + \sqrt{d_T^2(u_3) + 4^2} + \sqrt{4^2 + 2^2} \\
&+ \sqrt{d_T^2(u_4) + 1^2} - \sqrt{4^2 + d_T^2(u_4)} - \sqrt{4^2 + d_T^2(u_1)} - \sqrt{4^2 + d_T^2(u_2)} \\
&- \sqrt{4^2 + d_T^2(u_3)} - \sqrt{1^2 + 2^2} \\
&= \sqrt{4^2 + 2^2} + \sqrt{3^2 + 1^2} - \sqrt{4^2 + 3^2} - \sqrt{1^2 + 2^2} \\
&= 0.398 > 0.
\end{aligned}$$

By using Lemma 2.2.1, we obtain $SO(T^*) - SO(T) > 0$, which is a contradiction since T has maximum Sombor index. Hence, $m_{1,2} = 0$.

(ii) On contrary, assume that $m_{4,4} \neq 0$, that is, there exists $xy \in E(T)$ where $d_T(x) = d_T(y) = 4$. First we claim that $m_{1,3} \neq 0$,$m_{2,3} \neq 0$ and $m_{3,3} \neq 0$. On contrary, assume that $m_{1,3} = m_{2,3} = m_{3,3} = 0$. Using (i) in Equations (3.2c) and (3.2e) imply,

$$m_{1,4} = n_1 \tag{3.21}$$

$$m_{2,4} = 2n_2 \tag{3.22}$$

$$m_{3,4} = 3n_3 \tag{3.23}$$

Using Equations (3.21), (3.22) and (3.23) in (3.2f) we obtain $m_{4,4} = 4k - n_1 - 3n_3 - 2n_2$. By using values of n_1, n_2 and n_3 from Lemma 3.1.3 we get, $m_{4,4} = 4k - n + 1$, which further implies that $m_{4,4} \leq 0$. By Equation (3.11b), we have $n \geq 4k + 1$ which is a contradiction. Hence we get $m_{4,4} = 0$ when $m_{1,3} = m_{2,3} = m_{3,3} = 0$. Next there arise three cases to check $m_{4,4}$ when $m_{1,3} \neq 0$ or $m_{2,3} \neq 0$ or $m_{3,3} \neq 0$.

Case 1. If $m_{1,3} \neq 0$ then $m_{4,4} = 0$.
Proof is similar to Lemma 3.1.4(ii).

Case 2. If $m_{2,3} \neq 0$ then $m_{4,4} = 0$.
Proof is similar to Lemma 3.1.4(ii).

Case 3. If $m_{3,3} \neq 0$ then $m_{4,4} = 0$.
Proof is similar to Lemma 3.1.4(ii).

(iii) On contrary, assume that $m_{1,3} \neq 0$. Then, there exists $xy \in E(T)$ such that $d_T(x) = 1$ and $d_T(y) = 3$. This implies that $m_{1,4} < n_1 = \frac{n+k+1}{2}$. By Equation (3.11b), we get $m_{1,4} < \frac{5k-1+k+1}{2} + \frac{6k}{2} = 3k$. This indicates that there exists a vertex u with degree $d_T(u) = 4$ with at most 2 pendent vertices. The rest of the proof proceeds in a similar way as of Lemma 3.1.6 (iii).

(iv) On contrary, assume that $m_{2,4} \neq 2$. We know that $m_{2,4} \not> 2$ as $n_2 = 1$ by Lemma 3.1.3 (i). We assume that $m_{2,4} < 2$ and $u \in V(T)$ where $d_T(u) = 2$ where $\{u_1, u_2\} \in N_T(u)$. We consider the following cases:

Case 1: $d_T(u_1) = d_T(u_2) = 3$.

Let $d_T(x) = 4$, $x' \in N_T(x)$ and $d_T(x') \neq 1$. Without loss of generality, assume that there exist a $ux-$path containing uu_2 and $x'x$. Let T^* be another tree obtained from T, as follows:

$$T^* = T - uu_1 - uu_2 + xu + x'u + u_1u_2.$$

Then $T^* \in \mathcal{C}_2(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)$. Then we get

$$\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(x) + d_T^2(u)} + \sqrt{d_T^2(x') + d_T^2(u)} + \sqrt{d_T^2(u_1) + d_T^2(u_2)} \\
&- \sqrt{d_T^2(u) + d_T^2(u_1)} - \sqrt{d_T^2(u_2) + d_T^2(u)} - \sqrt{d_T^2(x) + d_T^2(x')} \\
&= \sqrt{4^2 + 2^2} + \sqrt{d_T^2(x') + 2^2} + \sqrt{3^2 + 3^2} - \sqrt{2^2 + 3^2} - \sqrt{3^2 + 2^2} \\
&- \sqrt{4^2 + d_T^2(x')} \\
&= \sqrt{4^2 + 2^2} + \sqrt{3^2 + 2^2} + \sqrt{3^2 + 3^2} - \sqrt{2^2 + 3^2} - \sqrt{3^2 + 2^2} \\
&- \sqrt{4^2 + 3^2} \\
&= 0.10 > 0.
\end{aligned}$$

By using Lemma 2.2.1, we obtain $SO(T^*) - SO(T) > 0$, which is a contradiction since T has maximum Sombor index.

Case 2. $d(u_1) = 4$ and $d_T(u_2) = 3$.

By (i), we know that $m_{1,2} = m_{2,2} = 0$ and by Lemma 3.1.3(ii), we know that $m_{1,4} = n_1 = \frac{n+k+1}{2}$. By Equation (3.11b) we get $\frac{5k+1}{2} < n_1 < \frac{6k-1}{2}$ or $2k < n_1 < 3k$. This indicates that there exists a degree 4 vertex that has exactly 3 pendant neighbors and there exists another degree 4 vertex that has at most 2 pendant neighbors.

Sub case 1: When u_1 has three pendant neighbors.

Let $d_T(y) = 4$ has at most two pendant neighbors. Let $\{y_1, y_2\} \in N_T(y)$ such that $d_T(y_1) \neq 1$ and $d_T(y_2) \neq 1$. As $m_{4,4} = 0$ by (ii), so $d_T(y_1) = d_T(y_2) = 3$. Without loss of generality, assume that there exist a u_1y_1-path containing u_2u and y_2y. Let T^* be another tree obtained from T, as follows:

$$T^* = T - yy_1 - yy_2 + uy + u_2y + y_1y_2.$$

Then $T^* \in \mathcal{C}_2(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)$. Then we get

$$\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(y) + d_T^2(u)} + \sqrt{d_T^2(u_2) + d_T^2(y)} + \sqrt{d_T^2(y_1) + d_T^2(y_2)} \\
&- \sqrt{d_T^2(y) + d_T^2(y_1)} - \sqrt{d_T^2(y_2) + d_T^2(y)} - \sqrt{d_T^2(u) + d_T^2(u_2)} \\
&= \sqrt{4^2 + 2^2} + \sqrt{4^2 + 3^2} + \sqrt{3^2 + 3^2} - \sqrt{2^2 + 3^2} - \sqrt{4^2 + 3^2} \\
&- \sqrt{4^2 + 3^2} \\
&= 0.10 > 0.
\end{aligned}$$

Here, we obtain $SO(T^*) - SO(T) > 0$, which is a contradiction since T has maximum Sombor index.

Sub case 2: When u_1 has at most two pendant neighbors.

Let $y \in N_T(u_1) \setminus \{u\}$ where $d_T(y) \neq 1$. Let $x \in N_T(v)$ where $d_T(v) = 1$ by (i) and (iii), $d_T(x) = 4$. Without loss of generality, assume that there exist a u_1v-path such that it contains u_1u. The maximality of path also implies that x has 3 pendant vertices. Let $x' \in N_T(x)$ and $d_T(x') \neq 1$. Using (ii) and Lemma 3.1.3 (i), we have $d_T(x') = d_T(y) = 3$ as $m_{4,4} = 0$. Let T^* be another tree obtained from T, as follows:

$$T^* = T - yu_1 - uu_2 - x'x + ux + u_1x' + yu.$$

Then $T^* \in C_2(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)$. Also

$$\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(x) + d_T^2(u)} + \sqrt{d_T^2(y) + d_T^2(u)} + \sqrt{d_T^2(u_1) + d_T^2(x')} \\
&- \sqrt{d_T^2(y) + d_T^2(u_1)} - \sqrt{d_T^2(u_2) + d_T^2(u)} - \sqrt{d_T^2(x') + d_T^2(x)} \\
&= \sqrt{4^2 + 2^2} + \sqrt{3^2 + 4^2} + \sqrt{3^2 + 3^2} - \sqrt{3^2 + 4^2} - \sqrt{2^2 + 3^2} \\
&- \sqrt{4^2 + 3^2} \\
&= 0.10 > 0.
\end{aligned}$$

Here, we obtain $SO(T^*) - SO(T) > 0$, which is a contradiction since T has maximum Sombor index. Hence, $m_{2,4} = 2$.

(v) By putting the values of n_1, n_2 and n_3 from Lemma 3.1.3 and $m_{1,2} = m_{2,2} = m_{1,3} =$

$m_{4,4} = 0$ and $m_{2,4} = 2$ in Equations (3.2c) to (3.2f), we obtain

$$\begin{aligned}
m_{3,4} &= \frac{7k - n - 5}{2}, \\
m_{1,4} &= \frac{n + k + 1}{2}, \\
m_{3,3} &= n - 4k - 1, \\
m_{2,3} &= 0.
\end{aligned}$$

This completes the proof. $\square$

Lemma 3.1.8. *Assume that a tree $T \in \mathcal{C}_3(n, k)$ has maximum Sombor index and $n-k$ is even. Then*

(i) $m_{1,2} = m_{2,2} = m_{2,3} = m_{2,4} = m_{4,4} = 0$

(ii) $m_{1,4} = 3k$

(iii) $m_{3,4} = k$, $m_{1,3} = \frac{n}{2} - \frac{5k}{2} + 1$, $m_{3,3} = \frac{n}{2} - \frac{3k}{2} - 2$.

Proof.

(i) This result is a direct outcome of Lemma 3.1.2(i) and 3.1.6(ii).

(ii) On contrary, assume that $m_{1,4} \neq 3k$. Then we have $m_{1,4} \ngtr 3k$ because if $m_{1,4} > 3k$, then tree is not connected. Now consider the case when $m_{1,4} < 3k$. If $m_{1,4} < 3k$, then $m_{1,3} > 0$. To prove this using contradiction, assume that $m_{1,3} \leq 0$, as edges cannot be negative so $m_{1,3} = 0$. Using $m_{1,2} = 0$ from (i) and Equation (3.2c), we get

$$m_{1,4} = n_1. \tag{3.24}$$

But, as we considered

$$m_{1,4} < 3k. \tag{3.25}$$

By Equations (3.24) and (3.25), we have

$$n_1 < 3k.$$

By Lemma 3.1.2 (ii), we get

$$\begin{aligned} \frac{n}{2} + \frac{k}{2} + 1 &< 3k, \\ n &< 5k - 2. \end{aligned}$$

This contradicts our statement that $T \in \mathcal{C}_3(n,k)$. Hence $m_{1,3} \neq 0$. This indicates there exists an edge $e = xy \in E(T)$ such that $d_T(x) = 1$ and $d_T(y) = 3$ with $\{y_1, y_2\} \in N_T(y)\backslash\{x\}$. Moreover, $m_{1,4} < 3k$ indicates that there exists a vertex u with $d_T(u) = 4$ with at most 2 pendent vertices. Let $\{u_1, u_2\} \in N_T(u)$ such that $d_T(u_1) \neq 1$ and $d_T(u_2) \neq 1$. Without loss of generality, assume there exists a $yu-$path containing yy_1 and u_1u. Now $d_T(u_2) = 3$ since by Part (i) we have $m_{2,4} = m_{4,4} = 0$. Let $\{s,t\} \in N_T(u_2)\backslash\{u\}$. Let T^* be another tree obtained from T, as follows:

$$T^* = T - u_2s - u_2z + xs + tx.$$

Then $T^* \in\mathcal{C}_3(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)\backslash\{u_2, x\}$ where $d_{T^*}(u_2) = d_T(u_2) - 2$ and $d_{T^*}(x) = d_T(x) + 2$. Then we get

$$\begin{aligned} SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(s) + (d_T(x)+2)^2} + \sqrt{d_T^2(t) + (d_T(x)+2)^2} \\ &+ \sqrt{(d_T(x)+2)^2 + d_T^2(y)} + \sqrt{d_T^2(u) + (d_T(u_2)-2)^2} \\ &- \sqrt{d_T^2(u) + d_T^2(u_2)} - \sqrt{d_T^2(u_2) + d_T^2(w)} \\ &- \sqrt{d_T^2(u_2) + d_T^2(t)} - \sqrt{d_T^2(x) + d_T^2(y)} \\ &= \sqrt{d_T^2(s) + 3^2} + \sqrt{d_T^2(t) + 3^2} + \sqrt{3^2+3^2} + \sqrt{4^2+1^2} \\ &- \sqrt{4^2+3^2} - \sqrt{3^2 + d_T^2(w)} - \sqrt{3^2 + d_T^2(z)} - \sqrt{1^2+3^2} \\ &= 0.20 > 0. \end{aligned}$$

Here, we obtain $SO(T^*) - SO(T) > 0$, which is a contradiction since T has maximum Sombor index. Hence, $m_{1,4} = 3k$.

(iii) By using the values of n_1 and n_3 from Lemma 3.1.2 (ii) and the values of edges obtained from (i) and (ii) in Equations (3.2c) to (3.2f), we get

$$\begin{aligned} m_{3,4} &= k, \\ m_{1,3} &= \frac{n}{2} - \frac{5k}{2} + 1, \\ m_{3,3} &= \frac{n}{2} - \frac{3k}{2} - 2. \end{aligned}$$

This finishes the proof. $\square$

Lemma 3.1.9. *Assume that a tree $T \in \mathcal{C}_3(n,k)$ has maximum Sombor index and $n-k$ is odd. Then*

(i) $m_{2,2} = m_{1,2} = m_{4,4} = 0$, $m_{2,3} = 1$

(ii) $m_{1,4} = 3k$

(iii) $m_{2,4} = 1$, $m_{1,3} = \frac{n-5k+1}{2}$, $m_{3,3} = \frac{n-3k-5}{2}$, $m_{3,4} = k-1$.

Proof.

(i) The proof of $m_{2,2} = m_{1,2} = m_{4,4} = 0$ is direct consequence of Lemma 3.1.3 (i) and 3.1.7 (i) and (ii). On contrary, assume that $m_{2,3} \neq 1$. Let $d_T(u) = 2$ and $\{u_1, u_2\} \in N_T(u)$. It can easily be seen that $m_{2,3} \not> 2$ as $n_2 = 1$ by Lemma 3.1.3(i). Further we will discuss two cases:

Case 1. $d(u_1) = d(u_2) = 3$.
This case is similar to Lemma 3.1.7 (iv).

Case 2. $d(u_1) = d(u_2) = 4$.
If $m_{2,4} = 2$, then $m_{1,3} \neq 0$. To prove this, assume that $m_{1,3} = 0$. Equation (3.2f) becomes $m_{1,4} = n_1 = \frac{n+k+1}{2}$. Using Equation (3.11c), we get $m_{1,4} > \frac{5k-3+k+1}{2} = 3k-1$. We obtain a contradiction since $n > 5k-3$ by Equation (3.11c). Assume that there exist an edge $xy \in E(T)$ such that $d_T(x) = 3$ and $d_T(y) = 1$. Without loss of generality, assume that there exist a $ux-$path such that u_1 does not lie on it. Let T^* be another tree obtained from T, as follows:

$$T^* = T - uu_1 + yu_1.$$

Then $T^* \in \mathcal{C}_3(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)\backslash\{u,y\}$ where $d_{T^*}(u) = d_T(u) - 1$ and $d_{T^*}(y) = d_T(y) + 1$. Then we get

$$\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{(d_T(y)+1)^2 + d_T^2(u_1)} + \sqrt{(d_T(u)-1)^2 + d_T^2(u_2)} \\
&+\sqrt{(d_T(y)+1)^2 + d_T^2(x)} - \sqrt{d_T^2(u) + d_T^2(u_1)} \\
&-\sqrt{d_T^2(u) + d_T^2(u_2)} - \sqrt{d_T^2(y) + d_T^2(x)} \\
&= \sqrt{2^2+4^2} + \sqrt{1^2+4^2} + \sqrt{2^2+3^2} - \sqrt{2^2+4^2} - \sqrt{2^2+4^2} \\
&-\sqrt{3^2+1^2} \\
&= 0.09 > 0.
\end{aligned}$$

Here, we obtain $SO(T^*) - SO(T) > 0$, which is a contradiction since T has maximum Sombor index. Hence $m_{2,3} = 1$.

(ii) On contrary, assume that $m_{1,4} \neq 3k$. $m_{1,4} \not> 3k$ because that would imply the existence of a vertex of degree 4 with four pendant neighbors. So, we just need to prove the case when $m_{1,4} < 3k$. First we claim that if $m_{1,4} < 3k$, then $m_{1,3} > 0$ for $n \geq 5k-3$, $k \geq 3$. On contrary, assume that $m_{1,3} = 0$.
Using $m_{1,2} = 0$ and $m_{1,3} = 0$ in Equation (3.2c) we get,

$$m_{1,4} = n_1. \tag{3.26}$$

But, as we assumed that,

$$m_{1,4} < 3k. \tag{3.27}$$

By Equations (3.26) and (3.27), we have

$$n_1 < 3k.$$

By Lemma 3.1.3 (ii), we get

$$\begin{aligned}
\frac{n+k+1}{2} &< 3k, \\
n &< 5k-1.
\end{aligned}$$

Here, we get contradiction since $T \in \mathcal{C}_3(n,k)$. Hence $m_{1,3} \neq 0$ and $m_{1,4} = 3k$.

(iii) By using the values of n_1, n_2 and n_3 from Lemma 3.1.3 and the values obtained from (i) and (ii) in Equations (3.2c) to (3.2f), we get

$$\begin{aligned} m_{2,4} &= 1, \\ m_{1,3} &= \frac{n-5k+1}{2}, \\ m_{3,3} &= \frac{n-3k-5}{2}, \\ m_{3,4} &= k-1. \end{aligned}$$

This completes the proof. □

3.2 Main Results

In this section, we find values of maximum Sombor index in $\mathcal{C}(n,k)$ and provide trees that attain these maximum values.

Theorem 3.2.1. *Let $T \in \mathcal{C}(n,k)$ and has maximum Sombor index. Then*

$$SO(T) = \begin{cases} \sqrt{17}n + (4\sqrt{2}-\sqrt{17})k - 4\sqrt{2} \\ \text{if } T \in \mathcal{C}(n,k) \text{ for } n = 3k+2 \text{ and } k \geq 1, \\ 3\sqrt{17} + 3\sqrt{5} \\ \text{if } T \in \mathcal{C}(n,k) \text{ for } n = 3k+3 \text{ and } k = 1, \\ (\frac{15+\sqrt{17}-8\sqrt{2}}{2})n + (\frac{\sqrt{17}-45+32\sqrt{2}}{2})k + \sqrt{17} + 4\sqrt{2} - 15 \\ \text{if } T \in \mathcal{C}_1(n,k) \text{ and } n-k \text{ is even}, \\ (\frac{15+\sqrt{17}-8\sqrt{2}}{2})n + (\frac{\sqrt{17}-45+32\sqrt{2}}{2})k + \frac{\sqrt{17}-45}{2} + 4\sqrt{2} + 4\sqrt{5} \\ \text{if } T \in \mathcal{C}_1(n,k) \text{ and } n-k \text{ is odd}, \\ (\frac{6\sqrt{2}+\sqrt{17}-5}{2})n + (\frac{35+\sqrt{17}-24\sqrt{2}}{2})k + \sqrt{17} - 5 - 3\sqrt{2} \\ \text{if } T \in \mathcal{C}_2(n,k) \text{ and } n-k \text{ is even}, \\ (\frac{6\sqrt{2}+\sqrt{17}-5}{2})n + (\frac{35+\sqrt{17}-24\sqrt{2}}{2})k + 4\sqrt{5} - 3\sqrt{2} + \frac{\sqrt{17}-25}{2} \\ \text{if } T \in \mathcal{C}_2(n,k) \text{ and } n-k \text{ is odd}, \\ (\frac{\sqrt{10}+3\sqrt{2}}{2})n + (5 + 3\sqrt{17} - \frac{5\sqrt{10}+9\sqrt{2}}{2})k + \sqrt{10} - 6\sqrt{2} \\ \text{if } T \in \mathcal{C}_3(n,k) \text{ and } n-k \text{ is even}, \\ (\frac{\sqrt{10}+3\sqrt{2}}{2})n + (5 + 3\sqrt{17} - \frac{5\sqrt{10}+9\sqrt{2}}{2})k + \sqrt{13} - 5 + \frac{2\sqrt{20}+\sqrt{10}}{2} \\ \text{if } T \in \mathcal{C}_3(n,k) \text{ and } n-k \text{ is odd}. \end{cases}$$

Proof. **Case 1.** For $T \in \mathcal{C}_1(n,k)$ and $n-k$ is even. By putting the values of $m_{u,v}$ for $(u,v) \in A$ from Lemma 3.1.4 in Equation (3.1), we obtain

$$SO(T) = \left(\frac{15+\sqrt{17}-8\sqrt{2}}{2}\right)n + \left(\frac{\sqrt{17}-45+32\sqrt{2}}{2}\right)k + \sqrt{17}+4\sqrt{2}-15.$$

Case 2. For $T \in \mathcal{C}_1(n,k)$ and $n-k$ is odd. By putting the values of $m_{u,v}$ for $(u,v) \in A$ from Lemma 3.1.5 in Equation (3.1), we obtain

$$SO(T) = \left(\frac{15+\sqrt{17}-8\sqrt{2}}{2}\right)n + \left(\frac{\sqrt{17}-45+32\sqrt{2}}{2}\right)k + \frac{\sqrt{17}-45}{2}+4\sqrt{2}+4\sqrt{5}.$$

Case 3. For $T \in \mathcal{C}_2(n,k)$ and $n-k$ is even. By putting the values of $m_{u,v}$ for $(u,v) \in A$ from Lemma 3.1.6 in Equation (3.1), we obtain

$$SO(T) = \left(\frac{6\sqrt{2}+\sqrt{17}-5}{2}\right)n + \left(\frac{35+\sqrt{17}-24\sqrt{2}}{2}\right)k + \sqrt{17}-5-3\sqrt{2}.$$

Case 4. For $T \in \mathcal{C}_2(n,k)$ and $n-k$ is odd. By putting the values of $m_{u,v}$ for $(u,v) \in A$ from Lemma 3.1.7 in Equation (3.1), we obtain

$$SO(T) = \left(\frac{6\sqrt{2}+\sqrt{17}-5}{2}\right)n + \left(\frac{35+\sqrt{17}-24\sqrt{2}}{2}\right)k + 4\sqrt{5}-3\sqrt{2}+\frac{\sqrt{17}-25}{2}.$$

Case 5. For $T \in \mathcal{C}_3(n,k)$ and $n-k$ is even. By putting the values of $m_{u,v}$ for $(u,v) \in A$ from Lemma 3.1.8 in Equation (3.1), we obtain

$$SO(T) = \left(\frac{\sqrt{10}+3\sqrt{2}}{2}\right)n + \left(5+3\sqrt{17}-\frac{5\sqrt{10}+9\sqrt{2}}{2}\right)k + \sqrt{10}-6\sqrt{2}.$$

Case 6. For $T \in \mathcal{C}_3(n,k)$ and $n-k$ is odd. By putting the values of $m_{u,v}$ for $(u,v) \in A$ from Lemma 3.1.9 in Equation (3.1), we obtain

$$SO(T) = \left(\frac{\sqrt{10}+3\sqrt{2}}{2}\right)n + \left(5+3\sqrt{17}-\frac{5\sqrt{10}+9\sqrt{2}}{2}\right)k + \sqrt{13}-5+\frac{2\sqrt{20}+\sqrt{10}}{2}.$$

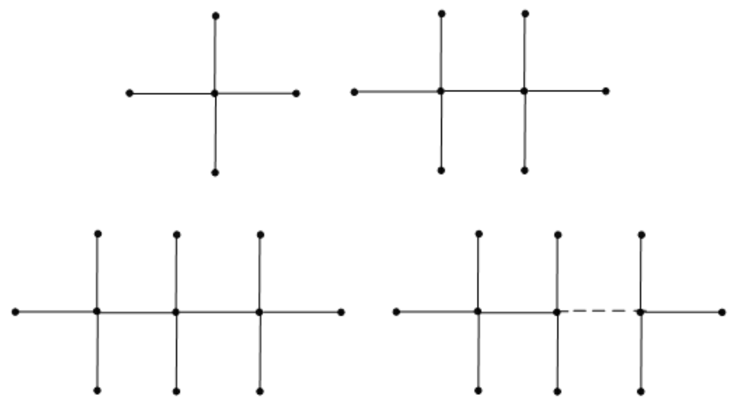

Figure 3.1: Trees with maximum Sombor index in $\mathcal{C}(n,k)$ when $n = 3k + 2$ and $k \geq 1$

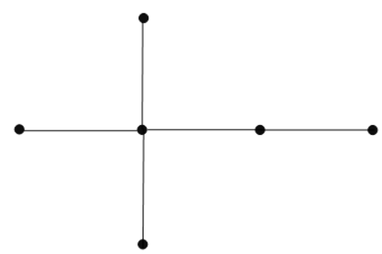

Figure 3.2: Tree with maximum Sombor index in $\mathcal{C}(n,k)$ when $n = 3k + 3$ for $k = 1$

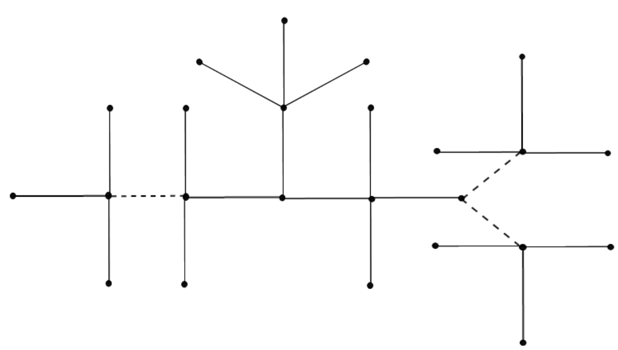

Figure 3.3: Tree with maximum Sombor index in $\mathcal{C}_1(n,k)$ when $n - k$ is even

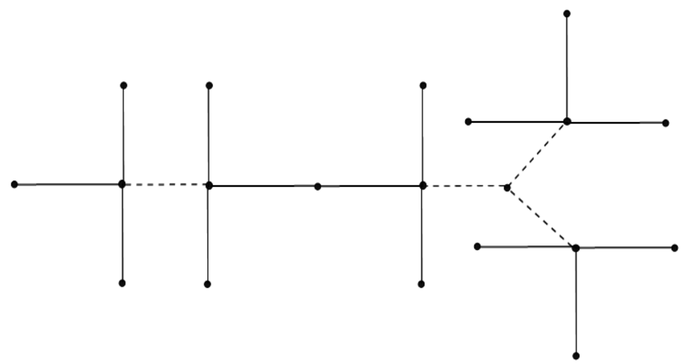

Figure 3.4: Tree with maximum Sombor index in $\mathcal{C}_1(n,k)$ when $n-k$ is odd

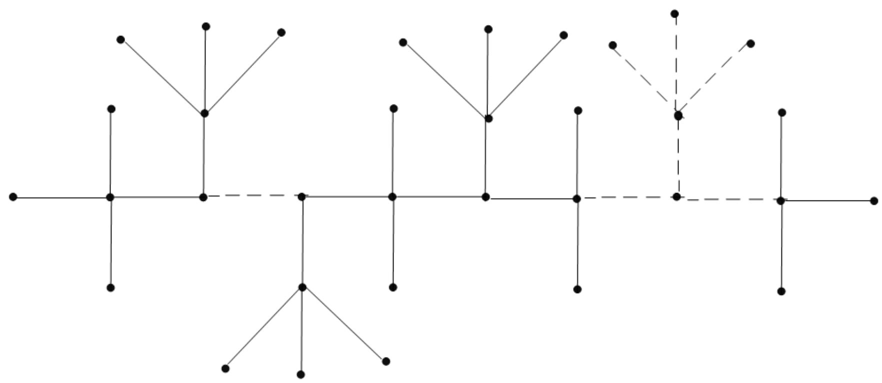

Figure 3.5: Tree with maximum Sombor index in $\mathcal{C}_2(n,k)$ when $n-k$ is even

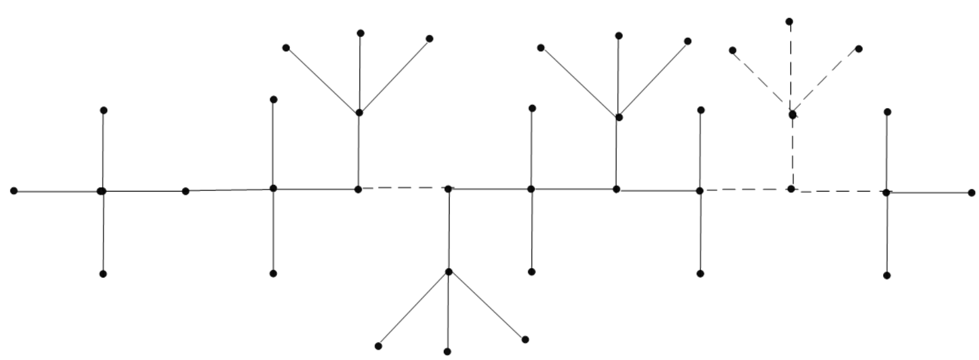

Figure 3.6: Tree with maximum Sombor index in $\mathcal{C}_2(n,k)$ when $n-k$ is odd

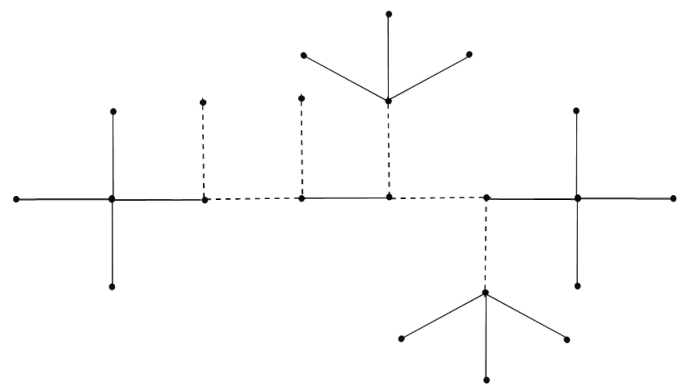

Figure 3.7: Tree with maximum Sombor index in $\mathcal{C}_3(n,k)$ when $n-k$ is even

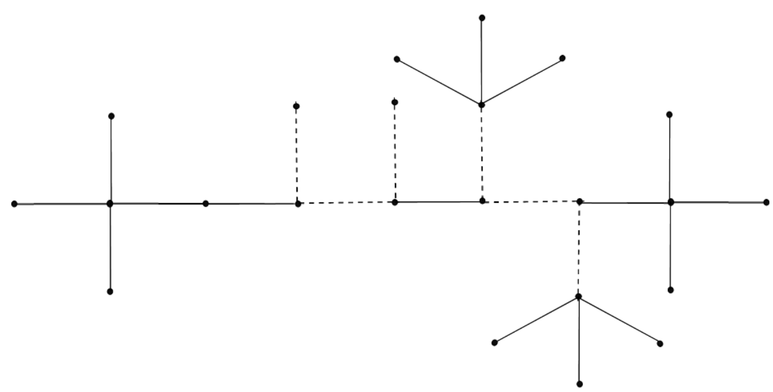

Figure 3.8: Tree with maximum Sombor index in $\mathcal{C}_3(n,k)$ when $n-k$ is odd

$\square$

Chapter 4

Minimum Sombor index of chemical trees with given vertices of maximum degree

Assume that $\mathcal{C}(n,k)$ be a class of chemical trees of order n and fixed vertex k of degree 4 for $k \geq 1$. In this chapter, we focus on determining the minimum Sombor index values of $\mathcal{C}(n,k)$.

4.1 Preliminaries

In this section, we provide some lemmas that are required in sequel.

Lemma 4.1.1. *Assume that a tree $T \in \mathcal{C}(n,k)$ has minimum Sombor index. Then*

(i) $n_3 = 0$

(ii) $n_1 = 2k+2$ *and* $n_2 = n - 3k - 2$.

Proof.

(i) On contrary, assume that there is a vertex u of degree 3 in T. Let $N_T(u) = \{u_1, u_2, u_3\}$. We will discuss two cases:

Case 1. The number of neighbors of u having degree 4 is 0 or 1. Without loss of generality, assume that $d_T(u_3) = 4$ and $1 \leq d_T(u_1), d_T(u_2) \leq 3$. Let x be the pendant vertex such that $x \notin N_T(u)$. Without loss of generality, assume that there exist a $u, x-$path and u_1 does not lie on it. Let $N_T(x) = \{x'\}$. Clearly, $2 \leq d_T(x') \leq 4$. Let T^* be another tree obtained from T, as follows:

$$T^* = T - u_1u + u_1x.$$

Then $T^* \in \mathcal{C}(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)\backslash\{u,x\}$ where $d_{T^*}(u) = d_T(u) - 1$ and $d_{T^*}(x) = d_T(x) + 1$. Then we get

$$\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(u_1) + (d_T(x)+1)^2} + \sqrt{(d_T(x)+1)^2 + d_T^2(x')} \\
&+ \sqrt{(d_T(u)-1)^2 + d_T^2(u_2)} + \sqrt{(d_T(u)-1)^2 + d_T^2(u_3)} \\
&- \sqrt{d_T^2(u_1) + d_T^2(u)} - \sqrt{d_T^2(x) + d_T^2(x')} \\
&- \sqrt{d_T^2(u) + d_T^2(u_2)} - \sqrt{d_T^2(u) + d_T^2(u_3)} \\
&= \sqrt{d_T^2(u_1) + 2^2} + \sqrt{2^2 + d_T^2(x')} + \sqrt{2^2 + d_T^2(u_2)} + \sqrt{2^2 + d_T^2(u_3)} \\
&- \sqrt{d_T^2(u_1) + 3^2} - \sqrt{1^2 + d_T^2(x')} - \sqrt{3^2 + d_T^2(u_2)} - \sqrt{3^2 + d_T^2(u_3)} \\
&= \sqrt{3^2 + 2^2} + \sqrt{2^2 + 2^2} + \sqrt{2^2 + 3^2} + \sqrt{2^2 + 4^2} - \sqrt{3^2 + 3^2} \\
&- \sqrt{1^2 + 2^2} - \sqrt{3^2 + 3^2} - \sqrt{3^2 + 4^2} \\
&= -1.20 < 0.
\end{aligned}$$

By using Lemmas 2.2.1 and 2.2.2, we obtain $SO(T^*) - SO(T) < 0$, which is a contradiction since T has minimum Sombor index.

Case 2. When 2 or 3 neighbors of u having degree four. Let $d(u_2) = d(u_3) = 4$. Without loss of generality, assume that there exist a $ux-$path, $d_T(x) = 1$ where $N_T(x) = x'$. Clearly, $2 \leq d_T(x') \leq 4$. Let T^* be another tree obtained from T, as follows:

$$T^* = T - u_2u - u_3u + ux + u_2u_3.$$

Then $T^* \in \mathcal{C}(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)\backslash\{u,x\}$ where $d_{T^*}(u) = d_T(u) - 1$ and $d_{T^*}(x) = d_T(x) + 1$. Then we get

$$
\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(u_2) + d_T^2(u_3)} + \sqrt{(d_T(x)+1)^2 + d_T^2(x')} \\
&+\sqrt{(d_T(u)-1)^2 + d_T^2(u_1)} + \sqrt{(d_T(u)-1)^2 + d_T^2(x) + 1} \\
&-\sqrt{d_T^2(u) + d_T^2(u_1)} - \sqrt{d_T^2(u) + d_T^2(u_2)} \\
&-\sqrt{d_T^2(u) + d_T^2(u_3)} - \sqrt{d_T^2(x) + d_T^2(x')} \\
&= \sqrt{4^2+4^2} + \sqrt{2^2 + d_T^2(x')} + \sqrt{2^2 + d_T^2(u_1)} + \sqrt{2^2+2^2} \\
&-\sqrt{3^2 + d_T^2(u_1)} - \sqrt{3^2+4^2} - \sqrt{3^2+4^2} - \sqrt{1^2 + d_T^2(x')} \\
&= \sqrt{4^2+4^2} + \sqrt{2^2+2^2} + \sqrt{2^2+4^2} + \sqrt{2^2+2^2} - \sqrt{3^2+4^2} \\
&-\sqrt{3^2+4^2} - \sqrt{3^2+4^2} - \sqrt{1^2+2^2} \\
&= -1.450 < 0.
\end{aligned}
$$

Using Lemmas 2.2.1 and 2.2.2, we obtain $SO(T^*)-SO(T) < 0$, which is a contradiction since T has minimum Sombor index. Therefore, $n_3 = 0$.

(ii) Using Part (i) in Equations (3.2b) and (3.2a), we get

$$n_1 + 2n_2 = 2n - 2 - 4k, \tag{4.1}$$

$$n_1 + n_2 = n - k. \tag{4.2}$$

Solving Equation (4.1) and (4.2) simultaneously, we get

$$
\begin{aligned}
n_1 &= 2k + 2, \\
n_2 &= n - 3k - 2.
\end{aligned}
$$

This completes the proof. □

Lemma 4.1.2. *Assume that a tree $T \in \mathcal{C}(n,k)$ has minimum Sombor index, then there does not appear any degree 2 vertex on any path connecting any two degree 4 vertices.*

Proof. On contrary, assume that there exist vertices $d_T(u) = d_T(v) = 4$, such that the path joining them has vertices of degree 2.

Case 1. When $d_T(u,v) = 2$. Let $x \in N_T(u,v)$. Clearly, $d_T(x) = 2$. Let $d_T(y) = 1$ and $N_T(y) = \{y'\}$. Clearly, $d_T(x) = 2$ and $2 \leq d_T(y') \leq 4$. We Let T^* be another tree obtained from T, as follows:

$$T^* = T - ux - vx + uv + xy.$$

Then $T^* \in \mathcal{C}(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)\backslash\{y,x\}$, where $d_{T^*}(x) = d_T(x) - 1$ and $d_{T^*}(y) = d_T(y) + 1$. Then we get

$$\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(u) + d_T^2(v)} + \sqrt{(d_T(y)+1)^2 + (d_T(x)-1)^2} \\
&+ \sqrt{(d_T(y)+1)^2 + (d_T^2(y')} - \sqrt{d_T^2(x) + (d_T^2(u)} \\
&- \sqrt{d_T^2(x) + d_T^2(v)} - \sqrt{d_T^2(y) + d_T^2(y')} \\
&= \sqrt{4^2+4^2} + \sqrt{2^2+1^2} + \sqrt{2^2 + (d_T^2(y')} - \sqrt{2^2+4^2} - \sqrt{2^2+4^2} \\
&- \sqrt{1^2 + d_T^2(y')} \\
&= \sqrt{4^2+4^2} + \sqrt{2^2+1^2} + \sqrt{2^2+2^2} - \sqrt{2^2+4^2} \\
&- \sqrt{2^2+4^2} - \sqrt{1^2+2^2} \\
&= -0.45 < 0.
\end{aligned}$$

By using Lemma 2.2.2, we obtain $SO(T^*) - SO(T) < 0$, which is a contradiction since T has minimum Sombor index.

Case 2. When $d_T(u,v) \geq 3$. Without loss of generality, assume that there exist a $uv-$path and $\{u_1, v_1\} \in N_T(u,v)$ lying on it, respectively. Clearly, $d_T(u_1) = d_T(v_1) = d_T(v_1') = 2$. Let $d_T(y) = 1$ and $N_T(y) = \{y'\}$. Clearly $2 \leq d_T(y') \leq 4$. Let T^* be another tree obtained from T, as follows:

$$T^* = T - vv_1 - uu_1 + uv + u_1y.$$

Then $T^* \in \mathcal{C}(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)\backslash\{y, v_1\}$ where $d_{T^*}(y) = d_T(y) + 1$ and $d_{T^*}(v_1) = d_T(v_1) - 1$. Then we get

$$
\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(u) + d_T^2(v)} + \sqrt{(d_T(y)+1)^2 + d_T^2(u_1)} \\
&+\sqrt{(d_T(v_1)-1)^2 + (d_T^2(v_1')} + \sqrt{(d_T(y)+1)^2 + (d_T^2(y')} \\
&-\sqrt{d_T^2(v_1) + d_T^2(v)} - \sqrt{d_T^2(v_1) + d_T^2(v_1')} \\
&-\sqrt{d_T^2(y) + d_T^2(y')} - \sqrt{d_T^2(u) + d_T^2(u_1)} \\
&= \sqrt{4^2+4^2} + \sqrt{2^2+2^2} + \sqrt{1^2+2^2} + \sqrt{2^2 + d_T^2(y')} \\
&-\sqrt{2^2+4^2} - \sqrt{2^2+2^2} - \sqrt{1^2 + d_T^2(y')} - \sqrt{4^2+2^2} \\
&= \sqrt{4^2+4^2} + \sqrt{2^2+2^2} + \sqrt{1^2+2^2} + \sqrt{2^2+2^2} - \sqrt{2^2+4^2} \\
&-\sqrt{2^2+2^2} - \sqrt{1^2+2^2} - \sqrt{4^2+2^2} \\
&= -0.45 < 0.
\end{aligned}
$$

By using Lemma 2.2.2, we obtain $SO(T^*) - SO(T) < 0$, which is a contradiction since T has minimum Sombor index. Hence, there does not appear any $d_T(2)$ on any path connecting any two $d_T(4)$. □

Consider the following subsets of $\mathcal{C}(n,k)$:

$$
\mathcal{C}_4(n,k) = \{T \in \mathcal{C}(n,k) : 3k+2 \le n \le 5k+4\}, \tag{4.3a}
$$

$$
\mathcal{C}_5(n,k) = \{T \in \mathcal{C}(n,k) : n > 5k+4\}. \tag{4.3b}
$$

Lemma 4.1.3. *Assume that a tree $T \in \mathcal{C}_4(n,k)$ has minimum Sombor index. Then*

(i) $m_{1,3} = m_{2,3} = m_{3,3} = m_{3,4} = 0$, $m_{4,4} = k-1$.

(ii) $m_{2,2} = 0$

(iii) $m_{1,2} = n-3k-2$, $m_{2,4} = n-3k-2$, $m_{1,4} = 5k+4-n$.

Proof.

(i) The proof of this part is direct consequence of Lemmas 4.1.1 (i) and 4.1.2.

(ii) On contrary, assume that T has an edge $uv \in E(T)$ where $d_T(u) = d_T(v) = 2$. First, we will show that if T has such an edge, then there must exist an edge $xy \in E(T)$ with $d_T(x) = 1$ and $d_T(y) = 4$. To prove this using contradiction, assume that there is no such edge that is, $m_{1,4} = 0$. Now, by solving Equations (3.2c) to (3.2f), for unknowns $m_{1,2}$, $m_{2,4}$ and $m_{2,2}$, we obtain the following,

$$\begin{aligned} m_{1,2} &= 2k+2, \\ m_{2,4} &= 2k+2, \\ m_{2,2} &= n-5k-4. \end{aligned}$$

This implies $m_{2,2} > 0$ if $n > 5k+4$ which is not possible because of Equation (4.1). This implies $m_{2,2} = 0$ if $m_{1,4} = 0$ which is in contradiction with our initial assumption that T has an edge uv with $d_T(u) = d_T(v) = 2$. Hence, if T has such edge, then there must exist an edge xy with $d_T(x) = 1$ and $d_T(y) = 4$. Without loss of generality, assume that there exist a $ux-$path containing v where $\{u_1, v_1\} \in N_T(u, v)$ lying on it, respectively. Let u_1 and v_1 be the neighbors of u and v respectively. Let T^* be another tree obtained from T, as follows:

$$T^* = T - uu_1 + u_1x.$$

Then $T^* \in \mathcal{C}_4(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)\backslash\{u, x\}$ where $d_{T^*}(u) = d_T(u) - 1$ and $d_{T^*}(x) = d_T(x) + 1$. Then we get

$$\begin{aligned} SO(T^*) - SO(T) &= \sqrt{d_T^2(u_1) + (d_T(x)+1)^2} + \sqrt{(d_T(u)-1)^2 + d_T^2(v)} \\ &+ \sqrt{(d_T(x)+1)^2 + d_T^2(y)} - \sqrt{d_T^2(u) + d_T^2(u_1)} - \sqrt{d_T^2(u) + d_T^2(v)} \\ &- \sqrt{d_T^2(x) + d_T^2(y)} \\ &= \sqrt{d_T^2(u_1) + 2^2} + \sqrt{1^2 + 2^2} + \sqrt{2^2 + 4^2} - \sqrt{2^2 + d_T^2(u_1)} \\ &- \sqrt{2^2 + 2^2} - \sqrt{2^2 + 4^2} \\ &= -0.59 < 0. \end{aligned}$$

Here, we obtain $SO(T^*) - SO(T) < 0$, which is a contradiction since T has minimum Sombor index. Hence, $m_{2,2} = 0$.

(iii) Now, solving the system of Equations (3.2c) to (3.2f) by using the values obtained from (i) and (ii) we get,

$$m_{1,2} = n - 3k - 2,$$
$$m_{2,4} = n - 3k - 2,$$
$$m_{1,4} = 5k + 4 - n.$$

This completes the proof. □

Lemma 4.1.4. *Assume that a tree $T \in \mathcal{C}_5(n,k)$ has minimum Sombor index. Then*

(i) $m_{1,3} = m_{2,3} = m_{3,3} = m_{3,4} = 0$ *,* $m_{4,4} = k - 1$

(ii) $m_{1,4} = 0$

(iii) $m_{1,2} = 2k + 2$*,* $m_{2,4} = 2k + 2$*,* $m_{2,2} = n - 5k - 4$*.*

Proof.

(i) The proof of this part is direct consequence of Lemmas 4.1.1 (i) and 4.1.2.

(ii) On contrary, assume that T has an edge $xy \in E(T)$ with $d_T(x) = 1, d_T(y) = 4$. Then, there must exist an edge $uv \in E(T)$ with $d_T(u) = d_T(v) = 2$. To prove this, on contrary assume that there is no such edge that is $m_{2,2} = 0$. By solving the Equations (3.2c), (3.2d), (3.2e) and (3.2f) we obtain the following,

$$m_{1,2} = n - 3k - 2,$$
$$m_{2,4} = n - 3k - 2,$$
$$m_{1,4} = 5k + 4 - n.$$

This implies $m_{1,4} > 0$ if $n < 5k + 4$ which is not possible because of Equation (4.3b). This implies $m_{1,4} = 0$ if $m_{2,2} = 0$ which is in contradiction with our initial assumption that T has an edge xy with $d_T(x) = 1$ and $d_T(y) = 4$. Hence, if $m_{1,4} \neq 0$, then $m_{2,2} \neq 0$ for $n > 5k + 4$. Let u_1 and v_1 be the neighbors of u and v respectively. Without loss of generality, assume that there exist a u,x-path containing v ending at some pendant vertex. Let T^* be another tree obtained from T, as follows:

$$T^* = T - uu_1 + u_1x.$$

Then $T^* \in \mathcal{C}_5(n,k)$. Clearly, $d_{T^*}(z) = d_T(z)$ for all $z \in V(T)\backslash\{x,u\}$ where $d_{T^*}(u) = d_T(u) - 1$ and $d_{T^*}(x) = d_T(x) + 1$. Then we get

$$\begin{aligned}
SO(T^*) - SO(T) \quad &= \sqrt{d_T^2(u_1) + (d_T(x)+1)^2} + \sqrt{(d_T(u)-1)^2 + d_T^2(v)} \\
&+ \sqrt{(d_T(x)+1)^2 + d_T^2(y)} - \sqrt{d_T^2(u) + d_T^2(u_1)} - \sqrt{d_T^2(u) + d_T^2(v)} \\
&- \sqrt{d_T^2(x) + d_T^2(y)} \\
&= \sqrt{d_T^2(u_1) + 2^2} + \sqrt{1^2 + 2^2} + \sqrt{2^2 + 4^2} - \sqrt{2^2 + d_T^2(u_1)} \\
&- \sqrt{2^2 + 2^2} - \sqrt{2^2 + 4^2} \\
&= -0.59 < 0.
\end{aligned}$$

Here, we obtain $SO(T^*) - SO(T) < 0$, which is a contradiction since T has minimum Sombor index. Hence, $m_{1,4} = 0$.

iii Now, solving the system of Equations (3.2c) to (3.2f) by using the values of edges obtained from (i) to (ii) we get,

$$\begin{aligned}
m_{1,2} \quad &= 2k + 2, \\
m_{2,4} \quad &= 2k + 2, \\
m_{2,2} \quad &= n - 5k - 4.
\end{aligned}$$

This completes the proof. □

4.2 Main Results

In this section, we will find values of minimum Sombor index in $\mathcal{C}(n,k)$ and provide trees that attain these minimum values.

Theorem 4.2.1. *Let $T \in \mathcal{C}(n,k)$ and has minimum Sombor index . Then*

$$SO(T) = \begin{cases} (3\sqrt{5}-\sqrt{17})n + (4\sqrt{2}-9\sqrt{5}+5\sqrt{17})k + 4\sqrt{17} - 6\sqrt{5} - 4\sqrt{2} \\ \quad \text{if } T \in \mathcal{C}_4(n,k) \\ 2\sqrt{2}n + (6\sqrt{5}-6\sqrt{2})k - 12\sqrt{2} + 6\sqrt{5} \\ \quad \text{if } T \in \mathcal{C}_5(n,k) \end{cases}$$

Proof. **Case 1.** For $T \in \mathcal{C}_4(n,k)$. By putting the values of $m_{u,v}$ for $(u,v) \in A$ from Lemma 4.1.3 in Equation (3.1), we obtain

$$SO(T) = (3\sqrt{5}-\sqrt{17})n + (4\sqrt{2}-9\sqrt{5}+5\sqrt{17})k + 4\sqrt{17} - 6\sqrt{5} - 4\sqrt{2}.$$

Case 2. For $T \in \mathcal{C}_5(n,k)$. By putting the values of $m_{u,v}$ for $(u,v) \in A$ from Lemma 4.1.4 in Equation (3.1), we obtain

$$SO(T) = 2\sqrt{2}n + (6\sqrt{5}-6\sqrt{2})k - 12\sqrt{2} + 6\sqrt{5}.$$

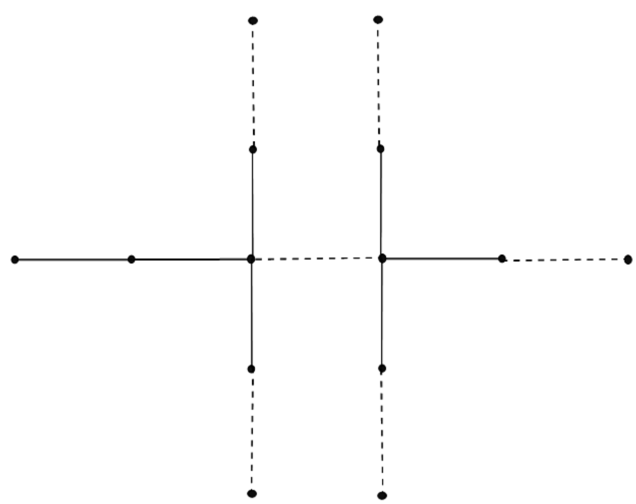

Figure 4.1: Tree with minimum Sombor index in $\mathcal{C}_4(n,k)$

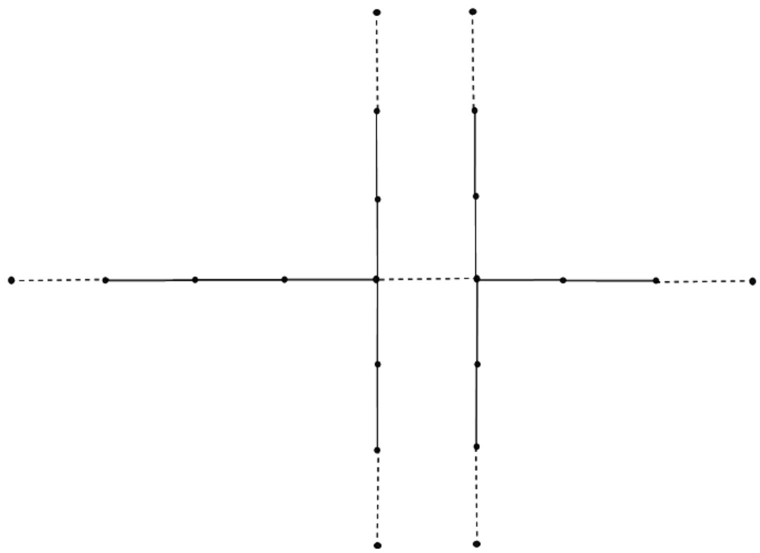

Figure 4.2: Tree with minimum Sombor index in $\mathcal{C}_5(n, k)$

$\square$

Chapter 5

Summary

In this thesis, the fundamental concepts of graph theory are discussed in detail. A brief introduction to chemical graph theory is given. Chemical graph theory aids in predicting the molecular properties by representing molecules in the form of graphs. This is usually done by finding topological indices, which are numerical parameters that remain unchanged under graph isomorphism. One of these topological indices is Sombor index. This thesis also encompasses determining the largest and the smallest values of Sombor index of chemical trees with given number of vertices of maximum degree.

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