General Sum-Connectivity Index and General Sombor Index of Chemical Trees with Given Order and Branching Vertices

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A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Mathematics (2024)

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I dedicate this thesis to my loving parents, honorable supervisor, respectable teachers, supportive seniors, and fellows for their unlimited guidance and support.

Acknowledgement

First, I want to thank **Allah Almighty** for showering His countless blessings on me and giving me health, ability, and strength to carry out this research work. Even though it was dif and only ificult for me to choose this work, Alhamdulillah He made everything easy for me, and I completed my dissertation fortuitously.

I prefer to present my heartiest appreciation to my supervisor, **Prof. Rashid Farooq** for his instruction throughout this work. I also appreciate him for listening to my problems keenly and discussing the pros and cons.

I would also like to thank my **seniors**, whose guidance and constant encouragement helped me get through the challenges throughout this journey.

I am grateful to my **parents** for their support, prayers, and their love that led me toward this marvelous success. If it was not for them I would not be able to stand firm in my life. They are the reason I did hard work because I never wanted to drag them down. I also want to thank my **siblings** for cheering me up and for their moral support.

Haleema Munir

Abstract

This thesis investigates the properties of graph indices with a focus on the extreme values of chemical trees with given order and branching vertices for the maximum general sum-connectivity index and maximum general Sombor index. For a graph G the general sum-connectivity and general Sombor indices are respectively given by

$$\chi_\sigma(G) = \sum_{pq \in E(G)} (d_G(p) + d_G(q))^\sigma \text{ and } \qquad \mathbb{SO}_\sigma(G) = \sum_{pq \in E(G)} (d_G^2(p) + d_G^2(q))^\sigma.$$

Here $d_G(p)$ represents the degree of a vertex p in a graph G and $E(G)$ is the edge set of G.

Graph indices are numerical quantities that capture specific structural attributes of graphs and have significant implications in various fields like chemistry, biology, and network analysis. The general sum-connectivity and general Sombor indices derived from the degrees of the vertices provide insights into the connectivity of graphs. Research on the general sum-connectivity index has been going on since 2010. However, the general Sombor index is a newly developed topological index introduced by Hu, X. and Zhong, L. in 2022, which gained extensive attention due to its vast applicability. In this thesis, we will determine the extremal values of general sum-connectivity and general Sombor indices of chemical trees with the given order n and branching vertices. By examining these indices, we aim to uncover patterns that enhance our understanding of graph structures and their applications.

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Chapter 1

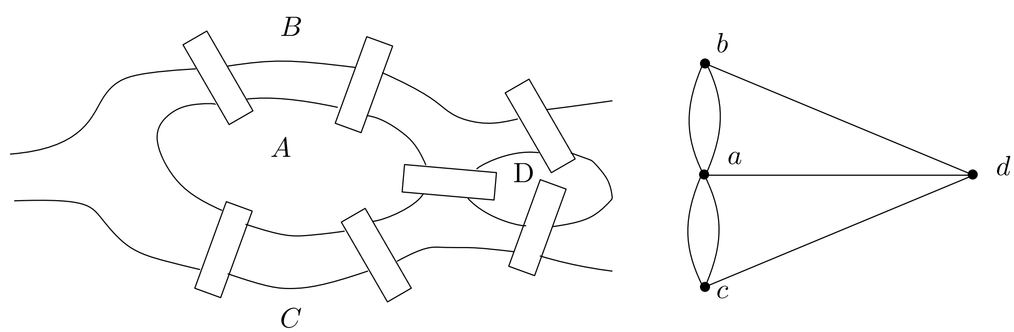
Introduction to graph theory

Graph theory is an important branch of mathematics due to its ability to model connections, which holds a significant role in computer science, chemistry, and network theory. To understand complex networks such as social interactions, transportation systems, and communication infrastructures, graphs provide a powerful framework. Using graphs to express these systems can unveil fundamental properties as they did hundreds of years ago.

1.1 Seven bridges of Königsberg problem

The concept of graph theory originated from the solution of "Königsberg's Seven Bridges" problem, a famous historical "puzzle" in mathematics and the theory of networks. Königsberg is a present-day Kaliningrad city in Russia, situated on both sides of the Pregel River, which divided the area into four landmasses; two islands and two mainlands connected by bridges. The challenge was to track down a walk within the city so that it crossed each bridge one time only and returned to the initial position.

The Swiss mathematician Leonhard Euler tackled the challenge in 1736 and presented his idea in a paper [18] titled "Solution of a problem relating to the geometry of position". He first approached the problem abstractly by representing the data visually as a graph by denoting the land areas as vertices and bridges as edges. However, he could not acquire the desired outcome. But, through this technique, he proved that it was impossible to find such a path because more than two vertices are connected to an odd number of vertices or attain odd degrees. Therefore, he proved that the problem could be solved if each vertex had an even degree, formulating the concept of the Eulerian circuit, which states that all vertices must have an even degree. This was only possible if the number of entrances and exits through the same bridge became equal. Thus, each landmass must have an even degree unless it is the starting or ending point. This result was similar to the Eulerian path, which states that the graph could have either zero or two vertices of odd degrees. Hence, the problem of Königsberg's Seven Bridges, could not be solved because each of the four vertices had odd degrees. However, this issue became the foundation of a new field, termed as *Graph Theory*. Here, it is important to note that Euler never used terms like graph, vertices, edges, path, or circuit. However, the basic structure of his work is similar to what we study today.



(a) Geographical Map (b) Graphical Representation

Figure 1.1: The Königsberg bridges

Almost a hundred years after Euler's work, Gustav Kirchhoff, a German physicist, used graphs to analyze electrical circuits in 1845, which led the foundation of new concepts like trees. He developed the famous Kirchhoff's

Theorem, which helps to find the order of spanning trees in an undirected connected graph. Later on, Arthur Cayley studied the properties of trees in the context of chemistry.

However, the term graph was first used by an English Mathematician J.J.Sylvester, in 1878 to show a connection between mathematical and chemical structures.

In the 20th century, mathematician Dénes Kőnig published the earliest textbook on graph theory in 1936, entitled "Theory of Finite and Infinite Graphs" [32].

Later on, new concepts were discovered that further enriched the field. These concepts may include coloring, matching, and planar graphs. Notably, the Four Color Theorem. It states that every planar graph can be colored with utmost four colors with no two neighbors sharing the same color. It was a conjecture till 1976 when Kenneth Appel and Wolfgang Haken proved it using computer knowledge [7].

In the 21st century, research on graph theory is increasing remarkably. Therefore, it is now a topic of interest for mathematicians and various other researchers from fields like chemistry, physics, and network topology are enthusiastically working on new problems and techniques.

1.2 Key terminologies in graph theory

In the area of mathematics, graphs hold a significant role. Particularly, to visualize the data, graphs are constructed. Hence, graph theory is the division of mathematics, in which we study the relations and connections between living or non-living objects. The objects are termed as vertices while the connection between them is represented by a straight line termed as an edge. A graph G is an unordered triplet of a vertex set, edge set, and an incidence function that designates two vertices $V(G)$ to each edge in the edge set $E(G)$.

The total vertices in $V(G)$ are termed as an order of a graph G and denoted by $n(G)$. The total edges present in $E(G)$ is termed as its size denoted by $m(G)$. Two vertices are adjacent in a graph G if they are endpoints of an edge e in G; otherwise, they are non-adjacent. In a simple graph, we denote an edge as $e = v_1v_2$. The total number of edges that are incident on a vertex v is termed as the degree of that vertex, denoted by $d_G(v)$ or $d_G(v)$. A sequence of numeric values that denotes the degrees of all the vertices of a graph G in descending order is termed the degree sequence of the graph G. A vertex with zero edge incident is labeled as an isolated vertex and a vertex whose degree is 1 is labeled as a pendent vertex.

The eccentricity of a vertex p is its maximum distance to any other vertex in G given by;

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

In a finite connected graph G, the eccentricity of each vertex of G is always finite.
The radius of a graph G is defined as

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

A disconnected graph therefore has infinite radius.
The diameter of a graph G is given by the formula

$$\mathrm{diam}(G) = \max\{e(p) \mid p \in V(G)\}.$$

A disconnected graph therefore has infinite diameter.
Within a graph G a vertex p is labeled as the central vertex of that graph G if $e(p) = \mathrm{rad}(G)$. The center of a graph G is a set of all the central vertices of the graph G.
Let G^* and G^{**} be two graphs. If $V(G^*) \supseteq V(G^{**})$ and $E(G^*) \supseteq E(G^{**})$, then the graph G^{**} is labeled as subgraph of G^*, denoted by $G^{**} \subseteq G^*$.
If $V(G^*) = V(G^{**})$, then G^{**} becomes a spanning subgraph.

1.3 Classification of graphs

Classification of graphs depends upon the structure of graphs. A graph with no loops or parallel edges is termed as a simple graph. A graph is referred to as a null graph if it has no edges. A graph is referred to as a trivial graph if it contains just one vertex. A graph is directed if its edges are represented by an arrow, otherwise, it is undirected.

An alternating sequence of a finite number of vertices and edges v_1, e_1, v_2, e_2,$\cdots$, v_i, e_i, v_{i+1} is termed as a walk so that endpoints of edge e_i are v_i and v_{i+1}. A walk without any repetition in edges is termed a trail. Fig 1.2 contains a walk v_1, e_9, v_5, e_5, v_6, e_{10}, v_2, e_2, v_3, e_3, v_4, e_4, v_5, e_5, v_6, e_6, v_7, e_7, v_8, e_8, v_1, e_1, v_2. In Fig 1.2 the sequence $v_1, e_1, v_2, e_2, v_3, e_3, v_4, e_4, v_5, e_9, v_1, e_8, v_8$, e_7, v_7, e_6, v_6, e_{10}, v_2 forms a trail. If the first and last vertices are the same in a walk, then it is labeled as a closed walk. A closed walk is termed a circuit if its vertices are allowed to repeat but its edges are not. In Fig 1.2, the sequence $v_1, e_9, v_5, e_5, v_6, e_{10}, v_2, e_2, v_3, e_3, v_4, e_4, v_5, e_5, v_6, e_6, v_7, e_7, v_8, e_8$ is a closed walk but not a circuit because edge e_5 is repeated. A circuit is referred as a simple circuit if its vertices are not allowed to repeat apart from the starting and ending vertex. In Fig 1.2, the sequence $v_1, e_1, v_2, e_{10}, v_6, e_5, v_5, e_9, v_1, e_1, v_2$ is a simple circuit.

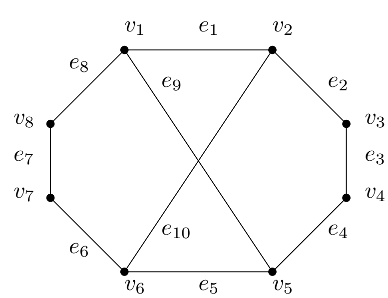


Figure 1.2: Graph G

A walk in which there is no repetition in vertices and edges is entitled as a path. A path of order n is represented by P_n. The total number of edges in P_n is termed as the length of P_n which is $n-1$. In Fig 1.3, the sequence $v_0, v_1, v_2, v_3, v_4, v_5$ is a path of length 5. The shortest path between two vertices is the path with the shortest length.

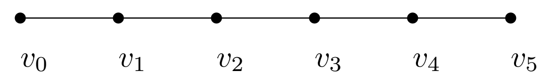


Figure 1.3: Path P_6

A loop in a graph G is an edge having the same endpoints. Two particular edges of a graph G which are incident on the same vertices are termed as parallel edges or multiple edges as shown in Fig 1.4.

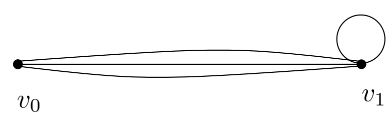
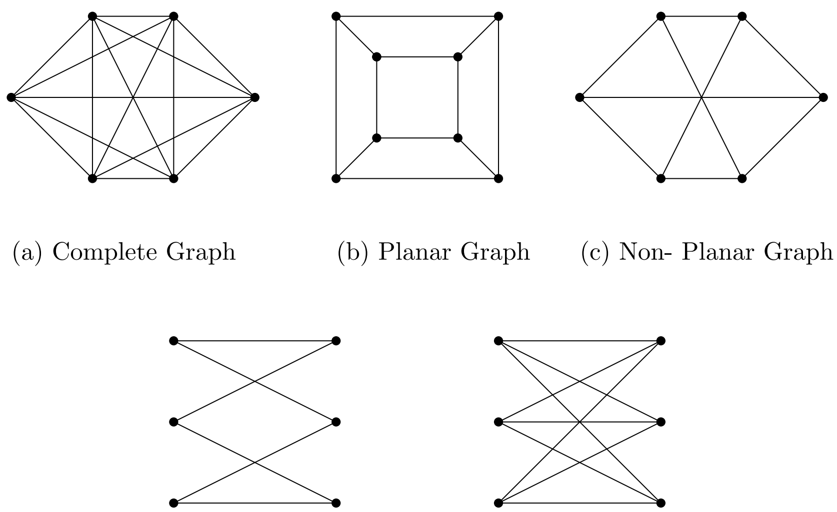


Figure 1.4: Loop and multiple edges

1.4 Some special kind of graphs

A simple graph G is termed as a complete graph if every two distinct vertices in G are adjacent by an edge. An n-vertex complete graph is represented by K_n. A graph B whose vertices may be divided into two disjoint sets, B_1 and B_2, and each edge of B connects a vertex in B_1 to a vertex in B_2 is termed a bipartite graph. If each vertex of one independent set of a bipartite graph is connected to each vertex of the other independent set then it is referred to a complete bipartite graph. If a graph is drawn in the plane in the way that no edge intersects the other except at the endpoints then it is referred to as a planar graph; otherwise, it is termed as non-planer.

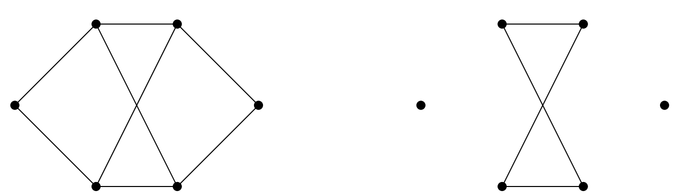


(a) Complete Graph (b) Planar Graph (c) Non- Planar Graph

(d) Bipartite Graph (e) Complete Bipartite Graph

Figure 1.5: Different kinds of graphs

A graph G is entitled as a regular graph if each vertex in G has the same degree. It may or may not be simple. A regular graph with degree k is referred to as an k-regular graph. In Fig 1.5, each graph is a regular graph. If at least one of a graph's vertices has a distinct degree from the other vertices then the graph is supposed to be irregular. An undirected graph G is referred to as a connected graph if there occurs a path between any two vertices of the graph G; otherwise, G is entitled as a disconnected graph.



(a) Connected Graph (b) Disconnected Graph

Figure 1.6: Connected and disconnected graphs

A cycle containing n vertices is a 2-regular simple and connected graph with $n \geq 3$. It is represented by C_n. A graph containing no cycle is termed as a forest. Fig 1.7 shows a cyclic and acyclic graph in a and b respectively. A connected graph which contains only one cycle, is entitled as a uni-cyclic graph. If a cycle has odd vertices then it is termed as an odd cycle otherwise an even cycle. A cycle of length three in a graph G is referred to as a triangle. A connected forest is entitled as a tree. A caterpillar is a tree that consists of a central "spine" path with pendents attached to it. A star is a tree with $n - 1$ pendent vertices and one central vertex. A double star is a tree with two non-pendent vertices.

Figure 1.7: Cyclic and acyclic graph

Table 1.1 shows the diameter and the radius for some well-known graphs for order n, where $n \geq 5$.

Graphs	Radius	Diameter
Complete graph $\mathbb{K}_n$	1	1
Path $\mathbb{P}_n$; if n is odd	$\frac{(n-1)}{2}$	$n - 1$
Path $\mathbb{P}_n$; if n is even	$\frac{n}{2}$	$n - 1$
Cycle $\mathbb{C}_n$; if n is odd	$\frac{(n-1)}{2}$	$\frac{(n-1)}{2}$
Cycle $\mathbb{C}_n$; if n is even	$\frac{n}{2}$	$\frac{n}{2}$
Star $\mathbb{S}_n$	1	2

Table 1.1

1.5 Representation of graphs as matrices

Graph representation using matrices is a powerful method to work with graphs in a mathematical and computational framework. There are two common ways to represent graphs:

(*i*) Adjacency matrix

(*ii*) Incidence matrix

The adjacency matrix of G is a square matrix of order n where each entry shows whether two vertices are adjacent in the graph. In simple graphs, data is usually represented in binary. In an adjacency matrix, two vertices are related by an edge, corresponding to 1. Otherwise, it is denoted by 0, if there is no form edge between the vertices.
The adjacency matrix of the graph given in Fig 1.2 is the following:

$$\begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

The incidence matrix of G is a matrix of order $m \times n$ where each row uses vertices and each column uses edges. Like an adjacency matrix, data is denoted by binary numbers. In the incidence matrix, vertices that are the endpoint of some edge correspond to 1. Otherwise, it is denoted by 0.

The incidence matrix of the graph given in Fig 1.2 is the following:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix}$$

Chapter 2

Topological indices and their analysis

In this chapter, we will discuss some topological indices. First, we will discuss the topic of chemical graph theory, in which these indices are applicable.

2.1 Chemical graph theory

In chemical graph theory, the vertices denote non-hydrogen atoms, while the edges denote the covalent bonds between the corresponding atoms. In particular, hydrocarbons are compounds formed by carbon and hydrogen atoms only. The chemical graphs of hydrocarbons denote the carbon skeleton of the molecule.

Chemical graph theory is a branch of mathematical chemistry that uses graph theory techniques to model the structure of molecules. It involves representing molecules as graphs, where atoms are assumed as vertices and chemical bonds are considered edges. This abstract representation allows chemists to predict the properties of molecules by offering insights into their structures.

The foundation of chemical graph theory can be traced back to the 19th century when pioneers like Arthur Cayley [11] started studying the properties of trees in the context of chemistry. Later, James Sylvester [42] made further significant contributions to the field by developing the connection between mathematics and chemistry laying the groundwork for modern chemical graph theory.

Chemical graph theory introduces various molecular descriptors, such as the Wiener index [46] and the Hosoya index [26], which quantify the structural features of molecules. These descriptors are essential in chemoinformatics for database searching and similarity analysis.

As the complexity of chemical systems continues to grow, the importance of chemical graph theory is likely to increase. By providing a deeper understanding of molecular structures and their properties, chemical graph theory will continue to play a crucial role in advancing the frontiers of science and technology.

2.2 Topological indices

In chemical graph theory, a molecular descriptor, also known as a topological graph index, is a mathematical equation or formula used to model the structure of a molecule, analyze mathematical values, and explore the physicochemical properties of a molecule. Thus, it provides a ground for cheaper and time-saving laboratory studies. That is why the topological index is important.

Topological indices play a significant role in QSAR study, where they help establish relationships between molecular structure and biological activity or other properties [10]. This predictive capability is crucial in QSAR studies for drug design, environmental chemistry, and material science. QSAR models built using topological indices provide insights into structure-activity relationships, guiding the design of new compounds with optimized properties.

In pharmaceutical research, topological indices aid in the identification of lead compounds and optimization of molecular structures for desired biological activities. They help prioritize compounds for synthesis and experimental testing [21].
These indices are also applied in environmental chemistry to assess the persistence, bioaccumulation, and toxicity of pollutants based on their molecular structure. In essence, topological indices provide a versatile framework for analyzing and interpreting chemical structures within the realm of graph theory. Their applications span from fundamental research in theoretical chemistry to practical applications in drug discovery, environmental science, and beyond, making them indispensable tools in modern chemical graph theory and computational chemistry. There are two most commonly used topological indices:
(1) distance-based topological indices.
(2) degree-based topological indices.

2.2.1 Distance-based topological indices

The "distance-based topological index" refers to a category of indices in graph theory and chemo-informatics that use pairwise distances between vertices in a molecular graph to quantify and predict various properties of molecules. These indices play a vital role in understanding molecular structure-function relationships and are widely applied in computational chemistry and related fields. The general formula of the distance-based topological index is given as

$$W(G) = \sum_{\{p,q\} \subseteq V(G)} F(d(p,\, q)). \tag{2.1}$$

In equation (2.1), $d(p,\, q)$ is the distance of the vertex p from the vertex q, and all of the ordered pair of vertices in the underlying chemical graph G are included in the summation, where $F(p, q)$ is some function having property $F(p, q) = F(q, p)$.

Several distance-based topological indices are used in graph theory and chemo-informatics, to describe molecular structures.

Harry Wiener [46] introduced the earliest known, Wiener Index in his seminal paper “Structural Determination of Paraffin Boiling Points” in 1947. Wiener was exploring the relationship between the molecular structure of alkanes and their boiling points. He found out that the sum of the distances among all pairs of carbon atoms in a molecule which he represented as a graph, could correspond to the boiling points of these compounds. Later on, a more generalized version of the Wiener Index was introduced, that considers not only the distances between pairs of vertices but also their squares. Hence, Serbian mathematician Ivan Gutman in 1993 introduced Hyper-Wiener Index [29].

Another one of famous indices is the Harary Index [39], named after Frank Harary, an American mathematician; considered one of the founders of modern graph theory. The index was introduced in 1959 and used in mathematical chemistry to describe the topology of chemical graphs. Although Frank Harary laid the groundwork for various graph theoretical concepts, it was Randić who applied these concepts to chemical graphs and formally introduced the Harary index in this context.

Balaban [13] introduced the J index in 1982 as a means to improve the discriminative power of topological indices for chemical graphs. He aimed to create an index that could more accurately reflect the complexity and connectivity of a molecule’s structure.

While existing indices like the Wiener [46] and Balaban J Indices [13] provided valuable information about molecular structures, there was a need for indices that could better capture the nuances of molecular branching and connectivity. The eccentric connectivity index [38] was introduced as a novel topological descriptor that combines information about vertex connectivity (degree) and vertex eccentricity. It was designed to provide a more detailed characterization of molecular structure by considering both the local and global aspects of vertex positions. Some more distance-based topological indices and their formula are given in Table 2.1.

2.2.2 Degree-based topological indices

The term "degree-based topological index" refers to a category of indices in graph theory used to describe molecular structure based on the degrees of vertices in the corresponding molecular graph. These indices are valuable tools in various fields for predicting and understanding the properties of molecules and materials. The general formula of a degree-based molecular descriptor is given as

$$T(G) = \sum_{pq \in E(G)} F(d_G(p), d_G(q)). \tag{2.2}$$

In equation (2.2), $d_G(p)$ is the degree of the vertex p, and all the pairs of adjacent vertices of the underlying chemical graph G are included in summation, where $F(p, q)$ is some function having property $F(p, q) = F(b, a)$.

Every degree-based topological index depends on the function $F(a, b)$, one can also associate a "reduced" index by replacing p with $p-1$ and q with $q-1$.

In contemporary mathematical chemistry, degree-based molecular descriptors, often known as topological indices, have been proposed and thoroughly investigated [30, 28].

The Zagreb indices were first introduced by the Croatian chemists Ivan Gutman and Nenad Trinajstć in 1972 [25]. They initially proposed these indices in the context of chemical graphs, which represent the structure of chemical compounds. Their pioneering work was published in a paper [25] titled "Graph Theory and Molecular Orbitals. Total π-Electron Energy of Alternant Hydrocarbons" in the journal Chemical Physics Letters. The paper introduced the first and second Zagreb indices as tools for predicting the total π-electron energy of alternant hydrocarbons. Variations of the Zagreb

indices, such as the Hyper-Zagreb index [44] and the multiplicative Zagreb indices [16], have also been introduced to capture more complex structural information.
The Randić index or connectivity index was defined by the Croatian chemist Milan Randić in 1975 [40]. The index was designed to capture the degree of branching in molecules. Randić proposed this index as a means to quantify the branching of the carbon-atom skeletons of alkanes and other molecular structures. Over time, several variants and extensions of the Randić index have been proposed to address different chemical and mathematical problems. Some of these include the generalized Randić index [43] and the sum-connectivity index [49]. The generalized Randić index introduces a parameter σ, where the original Randić index corresponds to $\sigma = \frac{1}{2}$.

The Iranian mathematician Ali Iranmanesh and Croatian chemist Ivan Gutman introduced the ABC index in 1998 [17]. They presented this index in their "On Atom-Bond Connectivity Index of Trees" paper published in Mathematical Chemistry (MATCH). Some variants include the modified ABC index, which adjusts the formula to better capture certain structural characteristics or to simplify calculations for larger and more complex chemical graphs.

The table below provides a list of these topological indices, however, it is not strictly complete. See [6] for more information.

Topological indices	Function $F(s,t)$
Wiener index [46]	$W(G) = \sum_{(s,t)\in V(G)} d_G(s,t)$
Hyper Wiener index [29]	$HW(G) = \frac{1}{2}\sum_{(s,t)\in V(G)}(d_G(s,t) + d_G(s,t)^2)$
First Zagreb index [25]	$M_1(G) = \sum_{st\in E(G)} d_G(s) + d_G(t)$
Second Zagreb index [25]	$M_2(G) = \sum_{st\in E(G)} d_G(s)d_G(t)$
Hyper Zagreb index [44]	$HM(G) = \sum_{st\in E(G)}(d_G(s) + d_G(t))^2$
Randić index [40]	$R(G) = \sum_{st\in E(G)} \frac{1}{\sqrt{d_G(s)d_G(t)}}$
Reciprocal Randić index [8]	$RR(G) = \sum_{st\in E(G)} \sqrt{d_G(s)d_G(t)}$
General sum-connectivity index [50]	$\chi_\sigma(G) = \sum_{st\in E(G)}(d_G(s) + d_G(t))^\sigma$
Atom Bond Connectivity index [17]	$ABC(G) = \sum_{st\in E(G)} \sqrt{\frac{d_G(s)+d_G(t)-2}{d_G(s)d_G(t)}}$
Harmonic index [48]	$H(G) = \sum_{st\in E(G)} \frac{2}{d_G(s)+d_G(t)}$
Forgotten index [24]	$F(G) = \sum_{s\in V(G)} d_G(s)^3$
Geometric-arithmetic index [19]	$GA(G) = \frac{2\sqrt{d_G(s)d_G(t)}}{d_G(s)+d_G(t)}$
Arithmetic-geometric index [45]	$AG(G) = \frac{d_G(s)+d_G(t)}{2\sqrt{d_G(s)d_G(t)}}$

Table 2.1

Now, we will do a detailed analysis of two important and popular topological indices, which are general sum-connectivity and general Sombor indices.

2.2.3 Analysis of general sum-connectivity index

Historically, the first vertex-degree-based topological indices were the Zagreb indices. The Zagreb indices, i.e., the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$, were originally defined in [31]. The generalized version of the first Zagreb index has also been introduced [33], known as the general first Zagreb index.

In 1975, Randić proposed a structural index called branching index [40] that nowadays is called Randić connectivity index. It is the most used topological index in QSPR and QSAR. The ordinary Randić connectivity index has been extended to the general Randić connectivity index defined in [9].

Recently, Zhou and Trinajstć [50] modified the concept of Randić index and obtained a new index, called the general sum-connectivity index and defined as follows:

$$\chi_\sigma(G) = \sum_{pq \in E(G)} (d_G(p) + d_G(q))^\sigma \tag{2.3}$$

where σ is a non-zero real number. General sum-connectivity index, generalizes both the sum-connectivity index and the first Zagreb index [49].

If $\sigma = \frac{-1}{2}$, then $\chi_{\frac{-1}{2}}(G) = \sum_{pq \in E(G)} \frac{1}{\sqrt{(d_G(p)+d_G(q))}}$, which is the sum-connectivity index defined by Zhou and Trinajstć [49].

If $\sigma = \frac{1}{2}$, then $\chi_{\frac{1}{2}}(G) = \sum_{pq \in E(G)} \sqrt{(d_G(p) + d_G(q))}$, which is the reciprocal sum-connectivity index.

If $\sigma = 1$, then $\chi_1(G) = \sum_{pq \in E(G)} (d_G(p) + d_G(q))$ becomes the first Zegreb index [23].

If $\sigma = -1$, then $2\chi_{-1}(G) = \sum_{pq \in E(G)} \frac{2}{(d_G(p)+d_G(q))}$ becomes the harmonic index [6].

If $\sigma = 2$, then $\chi_2(G) = \sum_{pq \in E(G)} (d_G(p) + d_G(q))^2$ gives hyper-Zegreb index [44].

If $\sigma = -2$, then $\chi_2(G) = \sum_{pq \in E(G)} \frac{1}{(d_G(p)+d_G(q))^2}$ gives reciprocal hyper-Zegreb index.

The general sum-connectivity index has been extensively used within mathematical chemistry. Akhtar et al. found the bounds for the general sum-connectivity index of composite graphs [3]. In another paper, the author determined the sharp bounds on the general sum-connectivity index of four operations on graphs [1]. More results of this index are presented in [15, 47, 37, 4, 2].

2.2.4 Analysis of general Sombor index

The Sombor index is a relatively new graph invariant in the field of mathematical chemistry and network theory.

$$\mathbb{SO}(G) = \sum_{pq \in E(G)} \sqrt{d_G^2(p) + d_G^2(q)} \tag{2.4}$$

where $d_G(p)$ represents the degree of vertex in a graph G.

Introduced by Ivan Gutman [22] in 2021, the Sombor index provides an innovative way to characterize and analyze the structural properties of graphs, particularly in the context of chemical graph theory, which is used to study molecular structures. Liu [34] studied the Sombor index of chemical graphs and their applications to the boiling point of benzenoid hydrocarbons. In [41] author worked on the chemical applicability of Sombor indices. Cruz [12] studied the Sombor index in the context of trees with at most three branch vertices. Moreover, extremal values of molecular trees for the Sombor index are studied by [14]. In [20] author finds the relationship between the Sombor index and some degree-based topological indices.

Motivated by the extensions of Randić and sum-connectivity indices and several works on the Sombor index, the general Sombor index was recently introduced in [27] and defined as

$$\mathbb{SO}_{\sigma}(G) = \sum_{xy \in E(G)} (d_G(x)^2 + d_G(y)^2)^{\sigma}, \tag{2.5}$$

where σ is the non-zero real number. If $\sigma = \frac{1}{2}$, then it is Sombor index, while for $\sigma = 1$, we get the forgotten index $F(G)$ [24]. Selvaraj et al. [36] study the general Sombor index for trees with given pendent vertices. However, further research on this index is still being done.

Chapter 3

Maximum general sum-connectivity index for chemical trees

In Chapter 2, we have done a detailed analysis of the general sum connectivity index, where we have traced its historical background and examined the significant research contributions that have shaped the index over the years. Building on the theoretical foundations in Section 2.2.3, this chapter introduces new research that extends the application and understanding of the general sum connectivity index. The findings discussed in this chapter are the result of original research, providing a new direction for future studies.
In Chapter 3, we mainly study the maximum values for the general sum-connectivity index in the class $\mathbb{CT}(n, b)$ of chemical trees of order n and b branching vertices. Before going into more detail, we first define the term chemical tree.

Definition 3.0.1. *A chemical tree is a tree in which the vertex has at most degree 4.*

For a chemical tree T, the general sum-connectivity index can also be written as:

$$\chi_\sigma(T) = \sum_{1\le i\le j\le 4} (i+j)^\sigma m_{ij}(T). \tag{3.1}$$

3.1 Preliminaries

In this section, we give some important lemmas that will be frequently used to prove the main result.

Lemma 3.1.1. *Let c, d and z are real numbers, where $d > c > 0$ and $z \ge 1$. Then*

(i) $\zeta_{c,d}(z) = (z+d)^\sigma - (z+c)^\sigma$ is strictly decreasing.

(ii) $\eta_{c,d}(z) = (z+c)^\sigma - (z+d)^\sigma$ is strictly increasing.

Proof. (i) We find that

$$\zeta'_{c,d}(z) = \sigma[(z+d)^{\sigma-1} - (z+c)^{\sigma-1}].$$

Note that $(z+d)^{\sigma-1} < (z+c)^{\sigma-1}$ for $\sigma \in (0,1)$. So, $\zeta'_{c,d}(z) < 0$. Thus, $\zeta_{c,d}(z)$ is a strictly decreasing function.

(ii) We find that

$$\eta'_{c,d}(z) = \sigma[(z+c)^{\sigma-1} - (z+d)^{\sigma-1}]$$

Note that $(z+c)^{\sigma-1} > (z+d)^{\sigma-1}$ for $\sigma \in (0,1)$. So, $\eta'_{c,d}(z) > 0$. Thus, $\eta_{c,d}(z)$ is a strictly increasing function.

This concludes the proof. □

Now, we will give an important lemma, the proof of which is trivial. This lemma will be used to prove the Lemmas 3.1.3 and 4.1.3.

Lemma 3.1.2. *Let p, q and σ are real numbers, where $p, q > 0$ and $p, q \neq \{1\}$. Then $\Lambda_{p,q}(\sigma) = p^\sigma + q^\sigma$ is strictly convex.*

Proof. We obtain $\Lambda''_{p,q}(\sigma) = (\ln p)^2 p^\sigma + (\ln q)^2 q^\sigma > 0$. Thus, $\Lambda_{p,q}(\sigma)$ is strictly convex. $\square$

Lemma 3.1.3. *For $\sigma \in (0, 1)$, we have*

(i) $2(7)^\sigma - 8^\sigma - 6^\sigma > 0$,

(ii) $2(6)^\sigma - 4^\sigma - 8^\sigma > 0$.

Proof. By Lemma 3.1.2, the functions

$$\Lambda_{\frac{8}{7},\frac{6}{7}}(\sigma) = (\frac{8}{7})^\sigma + (\frac{6}{7})^\sigma \text{ and } \Lambda_{\frac{4}{6},\frac{8}{6}}(\sigma) = (\frac{4}{6})^\sigma + (\frac{8}{6})^\sigma$$

are strictly convex for real number σ. We have

$$\Lambda_{\frac{8}{7},\frac{6}{7}}(0) = 2 = \Lambda_{\frac{8}{7},\frac{6}{7}}(1) \text{ and } \Lambda_{\frac{4}{6},\frac{8}{6}}(0) = 2 = \Lambda_{\frac{4}{6},\frac{8}{6}}(1).$$

(i). We obtain $\Lambda_{\frac{8}{7},\frac{6}{7}}(\sigma) < 2$ for $\sigma \in (0, 1)$. This implies $8^\sigma + 6^\sigma < 2(7)^\sigma$ for $\sigma \in (0, 1)$.
(ii). We obtain $\Lambda_{\frac{4}{6},\frac{8}{6}}(\sigma) < 2$ for $\sigma \in (0, 1)$. This implies $4^\sigma + 8^\sigma < 2(6)^\sigma$ for $\sigma \in (0, 1)$. $\square$

For a chemical tree T [35], the following results are well-known:

$$n = n_1(T) + n_2(T) + n_3(T) + n_4(T), \tag{3.2}$$

$$2(n-1) = n_1(T) + 2n_2(T) + 3n_3(T) + 4n_4(T). \tag{3.3}$$

$$\begin{aligned} 2m_{11}(T)+m_{12}(T)+m_{13}(T)+m_{14}(T)&=n_1(T),\\ m_{12}(T)+2m_{22}(T)+m_{23}(T)+m_{24}(T)&=2n_2(T),\\ m_{13}(T)+m_{23}(T)+2m_{33}(T)+m_{34}(T)&=3n_3(T),\\ m_{14}(T)+m_{24}(T)+m_{34}(T)+2m_{44}(T)&=4n_4(T). \end{aligned} \tag{3.4}$$

Now, in section 3.2, we will find the chemical trees with maximum χ_σ index for $\sigma \in (0,1)$ in $\mathbb{CT}(n,b)$ respectively. It is important to note that for a graph to be graphically feasible in $\mathbb{CT}(n,b)$, we consider $n \geq 2b+2$.

3.2 Chemical trees in $\mathbb{CT}(n,b)$ with maximum χ_σ index for $\sigma \in (0,1)$

In this section, we will determine the maximum χ_σ index for $\sigma \in (0,1)$ for chemical trees in $\mathbb{CT}(n,b)$. Here, we further classify $\mathbb{CT}(n,b)$ into two classes.

$$\begin{aligned} \mathbb{C}_1\mathbb{T}(n,b) = &\{T_1 \in \mathbb{CT}(n,b) \mid n \in \{4,5\} \text{ and } b=1\}\\ &\cup \{T_1 \in \mathbb{CT}(n,b) \mid n=13 \text{ and } b=4\}\\ &\cup \left\{T_1 \in \mathbb{CT}(n,b) \mid 2b+2 \leq n \leq \left\lfloor \frac{5b+5}{2} \right\rfloor \text{ and } b \geq 2\right\}\\ &\cup \left\{T_1 \in \mathbb{CT}(n,b) \mid \left\lceil \frac{5b+6}{2} \right\rceil \leq n \leq \left\lfloor \frac{8b+7}{3} \right\rfloor \text{ and } b \geq 6\right\}\\ &\cup \left\{T_1 \in \mathbb{CT}(n,b) \mid \left\lceil \frac{8b+8}{3} \right\rceil \leq n \leq 3b+2 \text{ and } b \geq 2\right\}.\\ \mathbb{C}_2\mathbb{T}(n,b) = &\{T_1 \in \mathbb{CT}(n,b) \mid n \geq 3b+3 \text{ and } b=1\}\\ &\cup \{T_1 \in \mathbb{CT}(n,b) \mid 3b+3 \leq n \leq 4b+1 \text{ and } b \geq 2\}\\ &\cup \{T_1 \in \mathbb{CT}(n,b) \mid n \geq 4b+2 \text{ and } b \geq 2\}. \end{aligned}$$

Now, we will prove the following lemmas to establish the main theorem.

Lemma 3.2.1. *Let $T_1 \in \mathbb{C}_1\mathbb{T}(n,b)$ be a chemical tree of order $2b+2 \leq n \leq$*

$3b+2$ *and* $b \geq 1$ *with maximum* χ_σ *index for* $\sigma \in (0,1)$. *Then*

(*i*) $n_2(T_1) = 0$,

(*ii*) $n_3(T_1) = 3b+2-n$, $n_1(T_1) = n-b$ *and* $n_4(T_1) = n-2b-2$.

Proof. (*i*) Contrarily, $n_2(T_1) \geq 1$. Then there occurs $w \in V(T_1)$ so that $d_{T_1}(w) = 2$. Assume $N_{T_1}(w) = \{w_1, w_2\}$. We claim that $n_3(T_1) \geq 1$. For if $n_3(T_1) = 0$, then we solve (3.2) and (3.3) simultaneously and note that $n_1(T_1) = 2 + 2n_4(T_1)$. Now, from (3.2), we note that $n \geq 3b+3$, which is a contradiction. Therefore, assume $x \in V(T_1)$ so that $d_{T_1}(x) = 3$ and $N_{T_1}(x) = \{x_1, x_2, x_3\}$. To avoid complexity, let x_1 and w_1 lie on x,w-path in T_1 (w_1 and x_1 may coincide with each other). Then we note that $2 \leq d_{T_1}(x_1) \leq 4$, $2 \leq d_{T_1}(w_1) \leq 4$, $1 \leq d_{T_1}(x_2) \leq 4$, $1 \leq d_{T_1}(x_3) \leq 4$ and $1 \leq d_{T_1}(w_2) \leq 4$. Now, we get $T_2 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n,b)$ from T_1 as:

$$T_2 = T_1 - ww_2 + xw_2.$$

This implies $d_{T_2}(x) = d_{T_1}(x) + 1 = 4$, $d_{T_2}(w) = d_{T_1}(w) - 1 = 1$ and $d_{T_2}(u) = d_{T_1}(u)$ for all $u \in V(T_1) \setminus \{x, w\}$. Now, we discuss the proof in two cases.

Case 1. If $wx \notin E(T_1)$, then to show $\chi_\sigma(T_2) - \chi_\sigma(T_1) > 0$, we note that

$$\begin{aligned}\chi_\sigma(T_2) - \chi_\sigma(T_1) &= \sum_{i=2}^{3}\Big((4 + d_{T_1}(x_i))^\sigma - (3 + d_{T_1}(x_i))^\sigma\Big)\\ &+ (4 + d_{T_1}(x_1))^\sigma - (3 + d_{T_1}(x_1))^\sigma\\ &+ (4 + d_{T_1}(w_2))^\sigma - (2 + d_{T_1}(w_2))^\sigma\\ &+ (1 + d_{T_1}(w_1))^\sigma - (2 + d_{T_1}(w_1))^\sigma.\end{aligned}$$

Since $\sigma > 0$, it follows that

$$\chi_\sigma(T_2) - \chi_\sigma(T_1) > (4 + d_{T_1}(w_2))^\sigma - (2 + d_{T_1}(w_2))^\sigma + (1 + d_{T_1}(w_1))^\sigma - (2 + d_{T_1}(w_1))^\sigma.$$

By using Lemma 3.1.1 (i) and (ii), we obtain

$$\chi_\sigma(T_2) - \chi_\sigma(T_1) > 8^\sigma - 6^\sigma + 3^\sigma - 4^\sigma = (1 - 2^\sigma)(3^\sigma - 4^\sigma).$$

Since $\sigma > 0$, it follows that $1 - 2^\sigma < 0$ and $3^\sigma - 4^\sigma < 0$. Hence, $\chi_\sigma(T_2) > \chi_\sigma(T_1)$.

Case 2. If $wx \in E(T_1)$, then to show $\chi_\sigma(T_2) - \chi_\sigma(T_1) > 0$, we note that

$$\chi_\sigma(T_2) - \chi_\sigma(T_1) = \sum_{i=2}^{3} \Big((4 + d_{T_1}(x_i))^\sigma - (3 + d_{T_1}(x_i))^\sigma \Big) + (4 + d_{T_1}(w_2))^\sigma - (2 + d_{T_1}(w_2))^\sigma.$$

Since $\sigma > 0$, it follows that $\chi_\sigma(T_2) - \chi_\sigma(T_1) > 0$. A contradiction arises from each case. Therefore, $n_2(T_1) = 0$.

(ii) By using Lemma 3.2.1 (i) in (3.2) and (3.3) and solving them simultaneously, we note that

$$\begin{aligned} n_1(T_1) &= n - b, \\ n_3(T_1) &= 3b + 2 - n, \\ n_4(T_1) &= n - 2b - 2. \end{aligned}$$

This concludes the proof. $\square$

Lemma 3.2.2. *Let $T_1 \in \mathbb{C}_1\mathbb{T}(n, b)$ be a chemical tree of order $2b + 2 \leq n \leq \left\lfloor \frac{5b+5}{2} \right\rfloor$ and $b \geq 2$ with maximum χ_σ index for $\sigma \in (0, 1)$. Then* *(i)* $m_{12}(T_1) = m_{22}(T_1) = m_{23}(T_1) = m_{24}(T_1) = 0$,

(ii) $m_{44}(T_1) = 0$,

(iii) $m_{14}(T_1) = 3n_4(T_1)$,

(iv) $m_{13}(T_1) = 5b - 2n + 6, \quad m_{34}(T_1) = n_4(T_1)$ *and* $m_{33}(T_1) = 3b - n + 1$.

Proof. (i) The proof follows instantly from Lemma 3.2.1 (i).

(ii) Contrarily, suppose that $xy \in E(T_1)$ so that $d_{T_1}(x) = 4 = d_{T_1}(y)$. We further claim that $m_{13}(T_1)$ and $m_{33}(T_1)$ can not be zero simultaneously. For if $m_{13}(T_1) = 0 = m_{33}(T_1)$, then by using Lemmas 3.2.1, 3.2.2 (i) in (3.4), we note that $m_{14}(T_1) = n - b$ and $m_{34}(T_1) = 9b + 6 - 3n$. Now, by substituting the values of $m_{14}(T_1), m_{34}(T_1)$ and Lemma 3.2.1 (ii) in (3.4), it follows that $m_{44}(T_1) = 3n - 8b - 7$. Since $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ has $n \leq \left\lfloor \frac{5b+5}{2} \right\rfloor$, which implies $m_{44}(T_1) \leq \frac{1-b}{2} < 0$, which is a contradiction. Hence, $m_{13}(T_1)$ and $m_{33}(T_1)$ cannot be zero simultaneously. Now, we further discuss the proof in two cases:

Case 1. If $m_{13}(T_1) \geq 1$, then let $uv \in E(T_1)$ so that $d_{T_1}(u) = 1$ and $d_{T_1}(v) = 3$. To avoid complexity, let x lie on u, y-path in T_1. Now, we get $T_2 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ from T_1 as:

$$T_2 = T_1 - xy - uv + vy + ux. \tag{3.5}$$

This implies $d_{T_2}(w) = d_{T_1}(w)$ for all $w \in V(T_1)$. Then to show $\chi_\sigma(T_2) - \chi_\sigma(T_1) > 0$, we note that

$$\chi_\sigma(T_2) - \chi_\sigma(T_1) > 5^\sigma - 4^\sigma + 7^\sigma - 8^\sigma.$$

Since by Lemma 3.1.1 (i), we have $\zeta_{3,0}(4) = 7^\sigma - 4^\sigma > 8^\sigma - 5^\sigma = \zeta_{3,0}(5)$. So, $\chi_\sigma(T_2) > \chi_\sigma(T_1)$, leads to a contradiction.

Case 2. If $m_{33}(T_1) \geq 1$, then let $uv \in E(T_1)$ so that $d_{T_1}(u) = 3 = d_{T_1}(v)$. To avoid complexity, let x and v lie on u, y-path in T_1. Now, to show $\chi_\sigma(T_2) - \chi_\sigma(T_1) > 0$, we perform the following calculation using the transformation (3.5):

$$\chi_\sigma(T_2) - \chi_\sigma(T_1) > 2(7)^\sigma - 8^\sigma - 6^\sigma > 0.$$

By Lemma 3.1.3 (i), a contradiction arises, implying $m_{44}(T_1) = 0$.

(iii) Contrarily, $m_{14}(T_1) \neq 3n_4(T_1)$. Now, we discuss the proof in two cases:
Case 1. If $m_{14}(T_1) > 3n_4(T_1)$, then we obtain a disconnected tree.
Case 2. Assume that $m_{14}(T_1) < 3n_4(T_1)$, this implies that there occurs $w \in V(T_1)$ of degree 4 with at least two non-pendent neighbors say, w_1 and w_2. From Lemma 3.2.1 (i), it is clear that $3 \leq d_{T_1}(w_1) \leq 4$, and $3 \leq d_{T_1}(w_2) \leq 4$. We further claim that if $m_{14}(T_1) < 3n_4(T_1)$, then $m_{13}(T_1) \geq 1$. On contrary, let $m_{13}(T_1) = 0$. From Lemmas 3.2.1 and 3.2.2 (i) in (3.4), we derive $m_{14}(T_1) = n - b$ or $n - b < 3n - 6b - 6$, implying $n > \frac{5b+6}{2}$. Since $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ has $n \leq \lfloor \frac{5b+5}{2} \rfloor$, which implies a contradiction. Therefore, we let $uv \in E(T_1)$ so that $d_{T_1}(u) = 3$ and $d_{T_1}(v) = 1$. To avoid complexity, assume that w_2 lies on w, u-path (w_2 may coincide with u). Now, we get $T_2 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ from T_1 as:

$$T_2 = T_1 - ww_1 - uv + wv + uw_1.$$

This implies $d_{T_2}(t) = d_{T_1}(t)$ for all $t \in V(T_1)$. Then to show $\chi_\sigma(T_2) - \chi_\sigma(T_1) > 0$, we note that

$$\chi_\sigma(T_2) - \chi_\sigma(T_1) = (1 + 4)^\sigma - (3 + 1)^\sigma + (3 + d_{T_1}(w_1))^\sigma - (4 + d_{T_1}(w_1))^\sigma.$$

By using Lemma 3.1.1 (ii), we obtain

$$\chi_\sigma(T_2) - \chi_\sigma(T_1) = 5^\sigma - 4^\sigma + 6^\sigma - 7^\sigma.$$

Since by Lemma 3.1.1 (i), we have $\zeta_{1,0}(4) = 5^\sigma - 4^\sigma > 7^\sigma - 6^\sigma = \zeta_{1,0}(6)$.

So, $\chi_\sigma(T_2) > \chi_\sigma(T_1)$, leads to a contradiction. Therefore, $m_{14}(T_1) = 3n_4(T_1)$.

(*iv*) By using Lemma 3.2.2 $(i) - (iii)$ in (3.4), we note that

$$m_{13}(T_1) = 5b - 2n + 6,$$
$$m_{34}(T_1) = n_4(T_1),$$
$$m_{33}(T_1) = 3b - n + 1.$$

This concludes the proof. □

Lemma 3.2.3. *Let $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ be a chemical tree of order $\left\lceil \frac{5b+6}{2} \right\rceil \leq n \leq \left\lfloor \frac{8b+7}{3} \right\rfloor$ and $b \geq 6$ with maximum χ_σ index for $\sigma \in (0, 1)$. Then*

(*i*) $m_{12}(T_1) = m_{22}(T_1) = m_{23}(T_1) = m_{24}(T_1) = 0$,

(*ii*) $m_{13}(T_1) = 0$,

(*iii*) $m_{14}(T_1) = n - b$,

(*iv*) $m_{44}(T_1) = 0$,

(*v*) $m_{34}(T_1) = 3n - 7b - 8$ *and* $m_{33}(T_1) = 8b + 7 - 3n$.

Proof. (*i*) The proof follows instantly from Lemma 3.2.1 (*i*).

(*ii*) Contrarily, $m_{13}(T_1) \geq 1$. Then $uv \in E(T_1)$ so that $d_{T_1}(v) = 1$ and $d_{T_1}(u) = 3$. Further, we claim that $m_{14}(T_1) < 3n - 6b - 6$. For if $m_{14}(T_1) > 3n - 6b - 6$, then we obtain a disconnected tree. Thus, we assume $m_{14}(T_1) = 3n - 6b - 6$. By using Lemma 3.2.3 (*i*) in (3.4), we note that $m_{13}(T_1) = 5b - 2n + 6$. Since $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ has $n \geq \left\lceil \frac{5b+6}{2} \right\rceil$, implying $m_{13}(T_1) \leq 5b - 2\left\lceil \frac{5b+6}{2} \right\rceil + 6 \leq 0$. This gives a contradiction. Thus, $m_{14}(T_1) < 3n - 6b - 6$. Now, we suppose that w is a vertex of degree 4 with at least two non-pendant neighbors, say w_2 and w_1. From Lemma 3.2.1, it is clear that $3 \leq d_{T_1}(w_1) \leq 4$ and $3 \leq d_{T_1}(w_2) \leq 4$.

To avoid complexity, assume that w_2 lies on w, u-path (w_2 and u may coincide). Now, by following transformation and calculations of Lemma 3.2.2 (iii), it follows that $m_{13}(T_1) = 0$.

(iii) By substituting Lemma 3.2.3 $(i) - (ii)$ in (3.4), we note that $m_{14}(T_1) = n - b$.

(iv) Contrarily, let $m_{44}(T_1) \geq 1$. Then $xy \in E(T_1)$ so that $d_{T_1}(x) = 4 = d_{T_1}(y)$. Further, we claim that $m_{33}(T_1) \geq 1$. For if $m_{33}(T_1) = 0$, then from Lemmas 3.2.3 $(i) - (iii)$ and (3.4), we note that $m_{34}(T_1) = 9b + 6 - 3n$. From Lemmas 3.2.1, 3.2.3 (iii) and $m_{34}(T_1) = 9b + 6 - 3n$, we derive $m_{44}(T_1) = 3n - 8b - 7$. Since $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ has $n \leq \left\lfloor \frac{8b+7}{3} \right\rfloor$, it follows that $m_{44}(T_1) \leq 3 \left\lfloor \frac{8b+7}{3} \right\rfloor - 8b - 7 \leq 0$, which is a contradiction. Thus, there occurs $uv \in E(T_1)$ so that $d_{T_1}(u) = 3 = d_{T_1}(v)$. To avoid complexity, assume that x and v lie on u, y-path. Now, by following the transformation and calculations from Case 2 of Lemma 3.2.2 (ii), we note that $m_{44}(T_1) = 0$.

(v) By substituting Lemma 3.2.1 and 3.2.3 $(i) - (iv)$ in (3.4), we note that

$$m_{34}(T_1) = 3n - 7b - 8,$$
$$m_{33}(T_1) = 8b + 7 - 3n.$$

This concludes the proof. □

Lemma 3.2.4. *Let $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ be a chemical tree of order $\left\lceil \frac{8b+8}{3} \right\rceil \leq n \leq 3b + 2$ and $b \geq 2$ with maximum χ_σ index for $\sigma \in (0, 1)$. Then*

(i) $m_{12}(T_1) = m_{22}(T_1) = m_{23}(T_1) = m_{24}(T_1) = 0$,

(ii) $m_{13}(T_1) = 0$,

(iii) $m_{14}(T_1) = n_1(T_1)$,

(iv) $m_{33}(T_1) = 0$,

(*v*) $m_{34}(T_1) = 3n_3(T_1)$ *and* $m_{44}(T_1) = 3n - 8b - 7$.

Proof. (*i*) The proof follows instantly from Lemma 3.2.1 (*i*).

(*ii*) Contrarily, let $m_{13}(T_1) \geq 1$. Then $uv \in E(T_1)$ so that $d_{T_1}(v) = 1$ and $d_{T_1}(u) = 3$. Further, we claim that $m_{14}(T_1) < 3n - 6b - 6$. For if $m_{14}(T_1) = 3n - 6b - 6$, then by using Lemma 3.2.4 (*i*) in (3.4), we note that $m_{13}(T_1) = 5b - 2n + 6$. Since $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n,b)$ has $n \geq \left\lceil \frac{8b+8}{3} \right\rceil$, implying $m_{13}(T_1) \leq \frac{-b+2}{3} \leq 0$, when $b \geq 2$. This gives a contradiction. Thus $m_{14}(T_1) < 3n - 6b - 6$. The remaining proof is similar to the proof of Lemma 3.2.3 (*ii*).

(*iii*) The proof is similar to proof of Lemma 3.2.3 (*iii*).

(*iv*) Contrarily, let $m_{33}(T_1) \geq 1$. Then $uv \in E(T_1)$ so that $d_{T_1}(u) = 3 = d_{T_1}(v)$. Further, we claim that $m_{44}(T_1) \neq 0$. For if $m_{44}(T_1) = 0$, then by Lemmas 3.2.1 and 3.2.4 (*i*) – (*iii*) in (3.4), we note that $m_{34}(T_1) = 3n - 7b - 8$. Then from Lemma 3.2.4 (*i*) – (*ii*) and $m_{34}(T_1) = 3n - 7b - 8$, it follows that $m_{33}(T_1) = 8b + 7 - 3n$. Since $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n,b)$ has $n \geq \left\lceil \frac{8b+8}{3} \right\rceil$, we get $m_{33}(T_1) \leq 8b + 7 - 3\left\lceil \frac{8b+8}{3} \right\rceil \leq 0$, which is a contradiction. Therefore, let $xy \in E(T_1)$ so that $d_{T_1}(x) = 4 = d_{T_1}(y)$. For simplicity, suppose that x and v lie on u,y-path. Now, by following the transformation and calculations of Case 2 of Lemma 3.2.2 (*ii*), we note that $m_{33}(T_1) = 0$

(*v*) By using Lemmas 3.2.1, 3.2.4 (*i*) – (*iv*) in (3.4), we note that

$$m_{34}(T_1) = 9b + 6 - 3n,$$
$$m_{44}(T_1) = 3n - 8b - 7.$$

This concludes the proof. □

Lemma 3.2.5. *Let* $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n,b)$ *be a chemical tree of order* 13 *and* $b = 4$ *with maximum* χ_σ *index for* $\sigma \in (0,1)$. *Then* (*i*) $m_{12}(T_1) = m_{22}(T_1) = m_{23}(T_1) = m_{24}(T_1) = 0$,

(*ii*) $n_1(T_1) = 9$, $n_3(T_1) = 1$, $n_4(T_1) = 3$,

(*iii*) $m_{33}(T_1) = 0$,

(*iv*) $m_{44}(T_1) = 0$,

(*v*) $m_{13}(T_1) = 0$, $m_{14}(T_1) = 9$ *and* $m_{34}(T_1) = 3$.

Proof. (*i*) The proof is the direct outcome of Lemma 3.2.1 (*i*).

(*ii*) The proof is the direct outcome of Lemma 3.2.1 (*ii*).

(*iii*) The proof is the direct outcome of Lemma 3.2.5 (*ii*).

(*iv*) Contrarily, let $m_{44}(T_1) \geq 1$. Then $xy \in E(T_1)$ so that $d_{T_1}(x) = 4 = d_{T_1}(y)$. We claim that $m_{13}(T_1) \neq 0$. Let $m_{13}(T_1) = 0$. Then by using Lemma 3.2.5 $(i) - (iii)$ in (3.4), we get $m_{14}(T_1) = 9$ and $m_{34}(T_1) = 3$. Now, using $m_{14}(T_1) = 9$ and $m_{34}(T_1) = 3$ in (3.4), we get $m_{44}(T_1) = 0$. Since $m_{44}(T_1) \geq 1$, we note that a contradiction. Hence, then there occurs $uv \in E(T_1)$ so that $d_{T_1}(u) = 1$ and $d_{T_1}(v) = 3$. To avoid complexity, assume that x lies on u, y-path in T_1. Now, by following the transformation and calculations from Case 1 of Lemma 3.2.2 (*ii*), we note that $m_{44}(T_1) = 0$.

(*v*) By using Lemmas 3.2.5 $(i) - (iv)$ in (3.4), we note that

$$\begin{aligned} m_{13}(T_1) &= 0, \\ m_{14}(T_1) &= 9, \\ m_{34}(T_1) &= 3. \end{aligned}$$

This concludes the proof. □

Lemma 3.2.6. *Let* $T_1 \in \mathbb{C}_2\mathbb{T}(n, b)$ *be a chemical tree of order* $n \geq 3b + 3$ *and* $b \geq 1$ *with maximum* χ_σ *index for* $\sigma \in (0, 1)$. *Then* *(i)* $n_3(T_1) = 0$,

(ii) $n_1(T_1) = 2b + 2$, $\quad n_2(T_1) = n - 3b - 2$ *and* $n_4(T_1) = b$.

Proof. (i) Contrarily, let $n_3(T_1) \geq 1$. Then there occurs $x \in V(T_1)$ so that $d_{T_1}(x) = 3$. Assume $N_{T_1}(x) = \{x_1, x_2, x_3\}$. Further, we claim that $n_2(T_1) \geq 1$. On the contrary, let $n_2(T_1) = 0$. Then from (3.2) and (3.3) we note that $n = 2 + 2b + n_4(T_1)$. Now, if $n_4(T_1) = 0$, we get $n = 2b + 2$ and if $n_4(T_1) \leq b$, we note that $n \leq 3b + 2$. In either case, we get a contradiction because $T_1 \in \mathbb{C}_2\mathbb{T}(n, b)$ has $n \geq 3b+3$. Thus, there occurs a vertex $w \in V(T_1)$ so that $d_{T_1}(w) = 2$. Assume $N_{T_1}(w) = \{w_1, w_2\}$. To avoid complexity, assume that x_1 and w_1 lie on x, w-path (w_1 and x_1 may coincide). This implies that $2 \leq d_{T_1}(x_1) \leq 4$, $2 \leq d_{T_1}(w_1) \leq 4$, $1 \leq d_{T_1}(x_2) \leq 4$, $1 \leq d_{T_1}(x_3) \leq 4$ and $1 \leq d_{T_1}(w_2) \leq 4$. The remaining proof is similar to the proof of Lemma 3.2.1 (i). Therefore, $n_3(T_1) = 0$.

(ii) By using Lemma 3.2.6 in (3.2) and (3.3), then by solving them simultaneously, we note that

$$n_1(T_1) = 2b + 2,$$
$$n_2(T_1) = n - 3b - 2,$$
$$n_4(T_1) = b.$$

This concludes the proof. $\square$

Lemma 3.2.7. *Let* $T_1 \in \mathbb{C}_2\mathbb{T}(n, b)$ *be a chemical tree of order* $n \geq 3b + 3$ *and* $b = 1$ *with maximum* χ_σ *index for* $\sigma \in (0, 1)$. *Then*

(i) $m_{13}(T_1) = m_{23}(T_1) = m_{33}(T_1) = m_{34}(T_1) = 0$,

(ii) $n_1(T_1) = 4$, $n_2(T_1) = n - 5$, $n_4(T_1) = 1$,

(iii) $m_{44}(T_1) = 0$

(iv) $m_{14}(T_1) = 3$,

(*v*) $m_{22}(T_1) = n - 6$, $m_{12}(T_1) = 1$ *and* $m_{24}(T_1) = 1$.

Proof. (*i*) The proof follows instantly from Lemma 3.2.6 (*i*).

(*ii*) By using $b = 1$ in Lemma 3.2.6 (*ii*), we note that $n_1(T_1) = 4$, $n_2(T_1) = n - 5$ and $n_4(T_1) = 1$.

(*iii*) This is an immediate outcome of Lemma 3.2.7 (*ii*).

(*iv*) Contrarily, let $m_{14}(T_1) \neq 3$. We discuss this in two cases.
Case 1. If $m_{14}(T_1) = 4$, we note that $T_1 \cong S_5$ This is not possible, because $n \geq 6$.
Case 2. Let $m_{14}(T_1) < 3$. Then there occurs $w \in V(T_1)$ with degree 4. Assume $N_{T_1}(w) = \{w_1, w_2, w_3, w_4\}$. Since $m_{14}(T_1) < 3$, it follows that w has at least two non-pendent neighbors. We assume that w_1 and w_2 are non-pendent neighbors of w. Let $x \notin N_{T_1}(w)$ be a pendent vertex, and x_1 be its neighbor. To avoid complexity, assume that w_2 lies on w, x-path (w_2 may coincide with x_1). Since $b = 1$, it implies $d_{T_1}(w_1) = 2 = d_{T_1}(w_2)$, and $d_{T_1}(x_1) = 2$. Now, we get $T_2 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ from T_1 as:

$$T_2 = T_1 - ww_1 - xx_1 + wx + x_1w_1$$

This implies $d_{T_2}(t) = d_{T_1}(t)$ for all $t \in V(T_1)$. Then to show $\chi_\sigma(T_2) - \chi_\sigma(T_1) > 0$, we note that

$$\chi_\sigma(T_2) - \chi_\sigma(T_1) = 5^\sigma - 6^\sigma + 4^\sigma - 3^\sigma.$$

Since by Lemma 3.1.1 (i), $\zeta_{2,0}(3) = 5^\sigma - 3^\sigma > 6^\sigma - 4^\sigma = \zeta_{2,0}(4)$. So, $\chi_\sigma(T_2) > \chi_\sigma(T_1)$, leads to a contradiction.

(*v*) By using Lemma 3.2.7 (*i*) − (*iv*) in (3.4), we note that

$$\begin{aligned} m_{22}(T_1) &= n-6, \\ m_{12}(T_1) &= 1, \\ m_{24}(T_1) &= 1. \end{aligned}$$

This concludes the proof. □

Lemma 3.2.8. *Let $T_1 \in \mathbb{C}_2\mathbb{T}(n,b)$ be a chemical tree of order $3b+3 \le n \le 4b+1$ and $b \ge 2$ with maximum χ_σ index for $\sigma \in (0,1)$. Then*

(*i*) $m_{13}(T_1) = m_{23}(T_1) = m_{33}(T_1) = m_{34}(T_1) = 0,$

(*ii*) $m_{12}(T_1) = 0,$

(*iii*) $m_{14}(T_1) = n_1(T_1)$

(*iv*) $m_{22}(T_1) = 0,$

(*v*) $m_{44}(T_1) = 4b+1-n$ *and* $m_{24}(T_1) = 2n-6b-4.$

Proof. (*i*) The proof follows instantly from Lemma 3.2.6 (*i*).

(*ii*) Contrarily, let $m_{12}(T_1) \ge 1$. Then $xx_1 \in E(T_1)$ so that $d_{T_1}(x_1) = 2$ and $d_{T_1}(x) = 1$. Since $b \ge 2$, it follows that T_1 has at least two branching vertices. Therefore, suppose that $v, w \in V(T_1)$ so that $d_{T_1}(w) = 4 = d_{T_1}(v)$. To avoid complexity, suppose that w lies on the x,v-path. Now, we discuss the proof in two cases:

Case 1. When $vw \in E(T_1)$. Then we get $T_2 \in \mathbb{C}_2\mathbb{T}(n,b)$ from T_1 as:

$$T_2 = T_1 - xx_1 - vw + vx_1 + wx.$$

This implies $d_{T_2}(u) = d_{T_1}(u)$ for all $u \in V(T_1)$. Then to show $\chi_\sigma(T_2) - \chi_\sigma(T_1) > 0$, we note that

$$\chi_\sigma(T_2) - \chi_\sigma(T) = 5^\sigma - 3^\sigma + 6^\sigma - 8^\sigma.$$

Since by Lemma 3.1.1 (i), $\zeta_{2,0}(3) = 5^\sigma - 3^\sigma > 8^\sigma - 6^\sigma = \zeta_{2,0}(6)$. So, $\chi_\sigma(T_2) > \chi_\sigma(T_1)$, leads to a contradiction.

Case 2. When $vw \notin E(T_1)$. Then v and w are connected by shortest path $P_{vw} = vw_s \cdots w_1 w$ and $d_{T_1}(w_s) = 2$, where $s \geq 1$. Now, we get $T_2 \in \mathbb{C}_2\mathbb{T}(n, b)$ from T_1 as:

$$T_2 = T_1 - ww_1 - xx_1 + wx + x_1 w_1.$$

This implies $d_{T_2}(t) = d_{T_1}(t)$ for all $t \in V(T_1)$. Now, the calculations are similar to Lemma 3.2.7 (iv), implying $m_{12}(T_1) = 0$.

(iii) By using Lemma 3.2.8 $(i) - (ii)$ in (3.4), we get $m_{14}(T_1) = n_1(T_1)$.

(iv) Contrarily, assume that $m_{22}(T_1) \neq 0$. Then $xy \in E(T_1)$ so that $d_{T_1}(x) = 2 = d_{T_1}(y)$. We further claim that if $m_{22}(T_1) \geq 1$, then $m_{44}(T_1) \geq 1$. For if $m_{44}(T_1) = 0$, then by using Lemmas 3.2.8 $(i) - (iii)$ in (3.4) we get $m_{24}(T_1) = 2b - 2$. From Lemmas 3.2.6, 3.2.8 $(i) - (ii)$ and $m_{24}(T_1) = 2b - 2$, we note that $m_{22}(T_1) = n - 4b - 1$. Since $T_1 \in \mathbb{C}_2\mathbb{T}(n, b)$ has $n \leq 4b + 1$, it follows that $m_{22}(T_1) \leq 0$. This contradicts the supposition. Thus, there occurs $uv \in E(T_1)$ so that $d_{T_1}(u) = 4 = d_{T_1}(v)$. To avoid complexity, assume that x and v lie on the y, u-path. Now, we get $T_2 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ from T_1 as:

$$T_2 = T_1 - uv - xy + ux + yv.$$

This implies $d_{T_2}(t) = d_{T_1}(t)$ for all $t \in V(T_1)$. Then to show $\chi_\sigma(T_2) - \chi_\sigma(T_1) > 0$, we note that

$$\chi_\sigma(T_2) - \chi_\sigma(T) = 2(6)^\sigma - 4^\sigma - 8^\sigma.$$

By using Lemma 3.1.3 (ii), a contradiction arises. Therefore, $m_{22}(T_1) = 0$.

(*v*) By using Lemma 3.2.8 $(i)-(iv)$ in (3.4), we get

$$m_{44}(T_1) = 4b + 1 - n,$$
$$m_{24}(T_1) = 2n - 6b - 4.$$

This concludes the proof. $\square$

Lemma 3.2.9. *Let $T_1 \in \mathbb{C}_2\mathbb{T}(n,b)$ be a chemical tree of order $n \geq 4b+2$ and $b \geq 2$ with maximum χ_σ index for $\sigma \in (0,1)$. Then*

(*i*) $m_{13}(T_1) = m_{23}(T_1) = m_{33}(T_1) = m_{34}(T_1) = 0,$

(*ii*) $m_{12}(T_1) = 0,$

(*iii*) $m_{14}(T_1) = 2b + 2.$

(*iv*) $m_{44}(T_1) = 0,$

(*v*) $m_{22}(T_1) = n - 4b - 1$ *and* $m_{24}(T_1) = 2b - 2.$

Proof. (*i*) The proof follows instantly from Lemma 3.2.6 (*i*).

(*ii*) The proof is similar to the proof of Lemma 3.2.8 (*ii*).

(*iii*) The proof is similar to the proof of Lemma 3.2.8 (*iii*).

(*iv*) Contrarily, let $m_{44}(T_1) \geq 1$. Then $xy \in E(T_1)$ so that $d_{T_1}(x) = 4 = d_{T_1}(y)$. We further claim that if $m_{44}(T_1) \geq 1$, then $m_{22}(T_1) \geq 1$. For if $m_{22}(T_1) = 0$, then by using Lemmas 3.2.6 and 3.2.9 $(i)-(ii)$ in (3.4), we get $m_{24}(T_1) = 2n - 6b - 4$. From Lemmas 3.2.6, 3.2.9 $(i)-(iii)$ and $m_{24}(T_1) = 2n - 6b - 4$, it follows that $m_{44}(T_1) = 4b + 1 - n$. Since $T_1 \in \mathbb{C}_2\mathbb{T}(n,b)$ has order $n \geq 4b+2$, it follows that $m_{44}(T_1) < 0$. This contradicts the supposition. Therefore, there occurs $xy \in E(T_1)$ so that $d_{T_1}(x) = 2 = d_{T_1}(y)$. To avoid complexity assume that x and v lie on y,u-path. By following the transformation and calculations from Lemma 3.2.8 (*iv*), we note that $m_{44}(T_1) = 0$.

(v) By using Lemma 3.2.9 $(i)-(iv)$ in (3.4), we get

$$\begin{aligned} m_{22}(T_1) &= n-4b-1, \\ m_{24}(T_1) &= 2b-2. \end{aligned}$$

This concludes the proof. $\square$

Theorem 3.2.1. *Let $\mathbb{CT}(n,b)$ be a chemical tree of order $n \geq 2b+2$ and $b \geq 1$ with maximum χ_σ index. Then*

$$\chi_\sigma(T_1) = \begin{cases} 3(4)^\sigma, & \textit{if } \ n = 4 \textit{ and } b = 1; \\ 4(5)^\sigma, & \textit{if } \ n = 5 \textit{ and } b = 1; \\ 9(5)^\sigma + 3(7)^\sigma, & \textit{if } \ n = 13 \textit{ and } b = 4; \\ n(3(5)^\sigma - 2(4)^\sigma + (7)^\sigma - (6)^\sigma) + b(-6(5)^\sigma + 5(4)^\sigma - 2(7)^\sigma \\ +3(6)^\sigma) - 6(5)^\sigma + 6(4)^\sigma - 2(7)^\sigma \\ +(6)^\sigma, & \textit{if } \ 2b+2 \leq n \leq \lfloor \frac{5b+5}{2} \rfloor \textit{ and } b \geq 2; \\ n((5)^\sigma + 3(7)^\sigma - 3(6)^\sigma) + b(-(5)^\sigma - 7(7)^\sigma + 8(6)^\sigma) \\ -8(7)^\sigma + 7(6)^\sigma, & \textit{if } \ \lceil \frac{5b+6}{2} \rceil \leq n \leq \lfloor \frac{8b+7}{3} \rfloor \textit{ and } b \geq 6; \\ n((5)^\sigma - 3(7)^\sigma + 3(8)^\sigma) + b(-(5)^\sigma + 9(7)^\sigma - 8(8)^\sigma) \\ +6(7)^\sigma - 7(8)^\sigma, & \textit{if } \ \lceil \frac{8b+8}{3} \rceil \leq n \leq 3b+2 \textit{ and } b \geq 2; \\ n(4)^\sigma + 3(5)^\sigma + (6)^\sigma + (3)^\sigma - 6(4)^\sigma, & \textit{if } \ n \geq 3b+3 \textit{ and } b = 1; \\ n(-(8)^\sigma + 2(6)^\sigma) + b(2(5)^\sigma + 4(8)^\sigma - 6(6)^\sigma) \\ +2(5)^\sigma + (8)^\sigma - 4(6)^\sigma, & \textit{if } \ 3b+3 \leq n \leq 4b+1 \textit{ and } b \geq 2; \\ n(4)^\sigma + b(2(5)^\sigma - 4(4)^\sigma + 2(6)^\sigma) + 2(5)^\sigma \\ -(4)^\sigma - 2(6)^\sigma, \ \textit{if } \ n \geq 4b+2 \textit{ and } b \geq 2. \end{cases}$$

Proof. **Case 1.** When $n = 4$ and $b = 1$. By using Lemma 3.2.1 in (3.1), we note that

$$\chi_\sigma(T_1) = 3(4)^\sigma.$$

Diagrammatically, we represent tree T_1 for this case as:

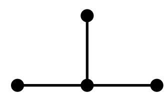


Figure 3.1: When $n = 4$ and $b = 1$

Case 2. When $n = 5$ and $b = 1$. By using Lemma 3.2.1 in (3.1), we note that

$$\chi_\sigma(T_1) = 4(5)^\sigma.$$

Diagrammatically, we represent tree T_1 for this case as:

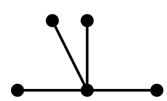


Figure 3.2: When $n = 5$ and $b = 1$

Case 3. When $n = 13$ and $b = 4$. By using Lemma 3.2.5 in (3.1), we note that

$$\chi_\sigma(T_1) = 9(5)^\sigma + 3(7)^\sigma,$$

where tree T_1 is given below:

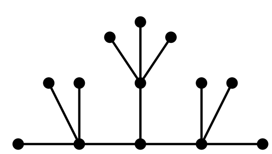


Figure 3.3: When $n = 13$ and $b = 4$

Case 4. When $2b+2 \leq n \leq \lfloor \frac{5b+5}{2} \rfloor$ and $b \geq 2$. By using Lemma 3.2.2 in (3.1), we note that

$$\begin{aligned}\chi_\sigma(T_1) &= n(3(5)^\sigma - 2(4)^\sigma + (7)^\sigma - (6)^\sigma) + b(-6(5)^\sigma + 5(4)^\sigma - 2(7)^\sigma + 3(6)^\sigma) \\ &\quad - 6(5)^\sigma + 6(4)^\sigma - 2(7)^\sigma + (6)^\sigma.\end{aligned}$$

Diagrammatically, we represent trees for this case as

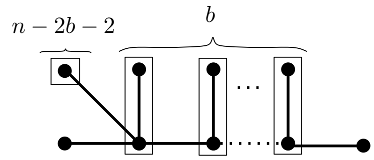


Figure 3.4: When $2b+2 \leq n \leq 2b+3$ and $b \geq 1$

and

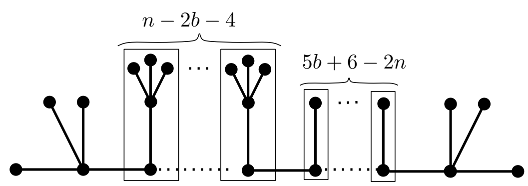


Figure 3.5: When $2b+4 \leq n \leq \lfloor \frac{5b+5}{2} \rfloor$ and $b \geq 2$

Case 5. When $\lceil \frac{5b+6}{2} \rceil \leq n \leq \lfloor \frac{8b+7}{3} \rfloor$ and $b \geq 6$. By using Lemma 3.2.3 in (3.1), we note that

$$\chi_\sigma(T_1) = n((5)^\sigma + 3(7)^\sigma - 3(6)^\sigma) + b(-(5)^\sigma - 7(7)^\sigma + 8(6)^\sigma) - 8(7)^\sigma + 7(6)^\sigma,$$

where tree T_1 is given below:

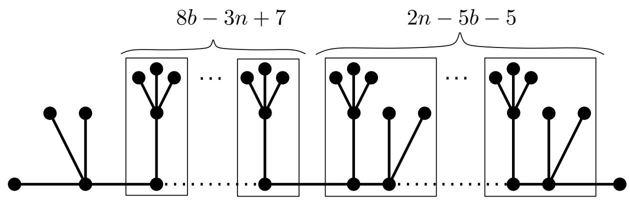


Figure 3.6: When $\lceil \frac{5b+6}{2} \rceil \leq n \leq \lfloor \frac{8b+7}{3} \rfloor$ and $b \geq 6$

Case 6. When $\lceil \frac{8b+8}{3} \rceil \leq n \leq 3b+2$ and $b \geq 2$. By using Lemma 3.2.4 in (3.1), we note that

$$\chi_\sigma(T_1) = n((5)^\sigma - 3(7)^\sigma + 3(8)^\sigma) + b(-(5)^\sigma + 9(7)^\sigma - 8(8)^\sigma) + 6(7)^\sigma - 7(8)^\sigma,$$

where tree T_1 is given below:

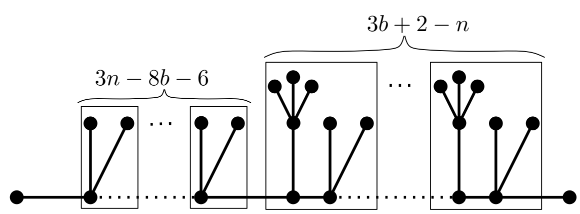


Figure 3.7: When $\lceil \frac{8b+8}{3} \rceil \leq n \leq 3b+2$ and $b \geq 2$

Case 7. When $n \geq 3b+3$ and $b = 1$. By using Lemma 3.2.7 in (3.1), we note that

$$\chi_\sigma(T_1) = n(4)^\sigma + 3(5)^\sigma + (6)^\sigma + (3)^\sigma - 6(4)^\sigma,$$

where tree T_1 is given below:

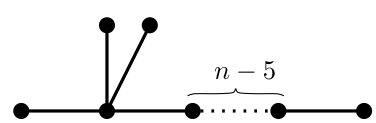


Figure 3.8: When $n \geq 3b+3$ and $b = 1$

Case 8. When $3b+3 \leq n \leq 4b+1$ and $b \geq 2$. By using Lemma 3.2.8 in (3.1), we note that

$$\chi_\sigma(T_1) = n(-(8)^\sigma + 2(6)^\sigma) + b(2(5)^\sigma + 4(8)^\sigma - 6(6)^\sigma) + 2(5)^\sigma + (8)^\sigma - 4(6)^\sigma,$$

where tree T_1 is given below:

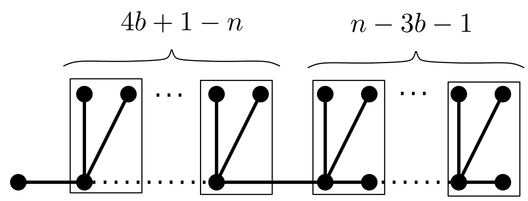


Figure 3.9: When $3b+3 \leq n \leq 4b+1$ and $b \geq 2$

Case 9. When $n \geq 4b+2$ and $b \geq 2$. By using Lemma 3.2.9 in (3.1), we note that

$$\chi_\sigma(T_1) = n(4)^\sigma + b(2(5)^\sigma - 4(4)^\sigma + 2(6)^\sigma) + 2(5)^\sigma - (4)^\sigma - 2(6)^\sigma,$$

where tree T_1 is given below:

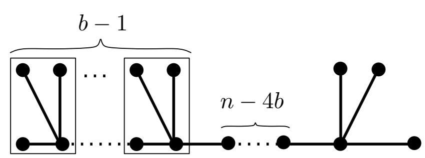


Figure 3.10: When $n \geq 4b+2$ and $b \geq 2$

This concludes the proof. $\square$

Chapter 4

Maximum general Sombor index for chemical trees

In this chapter, we introduce the general Sombor index, a novel graph invariant that extends the capabilities of the traditional Sombor index. While Chapter 2, provided a comprehensive analysis of established graph indices, this chapter presents original research that pushes the boundaries of graph theory by developing and exploring the general Sombor index. In this chapter, we mainly focus on the maximum values for the general Sombor index in the class $\mathbb{CT}(n, b)$ of chemical trees of order n and b branching vertices for $\sigma \in (0, 1)$. Our results generalize the finding on the Sombor index presented in [5], which serves as the special case of the general Sombor index when $\sigma = \frac{1}{2}$.

For a chemical tree T, the general Sombor index can also be written as:

$$\mathbb{SO}_\sigma(T) = \sum_{1 \le i \le j \le 4} (i^2 + j^2)^\sigma m_{ij}(T). \tag{4.1}$$

4.1 Preliminaries

In this section, we give some important lemmas that will be frequently used to prove the main result.

Lemma 4.1.1. *Let c, d and z are real numbers, where $d > c > 0$ and $z \geq 1$. Then*

(i) $\psi_{c,d}(z) = (z^2 + d^2)^\sigma - (z^2 + c^2)^\sigma$ *is strictly decreasing.*

(ii) $\gamma_{c,d}(z) = (z^2 + c^2)^\sigma - (z^2 + d^2)^\sigma$ *is strictly increasing.*

Proof. (i) We find that

$$\psi'_{c,d}(z) = 2\sigma z[(z^2 + d^2)^{\sigma-1} - (z^2 + c^2)^{\sigma-1}].$$

Note that $(z^2 + d^2)^{\sigma-1} < (z^2 + c^2)^{\sigma-1}$ for $\sigma \in (0, 1)$. So, $\psi'_{c,d}(z) < 0$. Thus, $\psi_{c,d}(z)$ is a strictly decreasing function.

(ii) We find that

$$\gamma'_{c,d}(z) = 2\sigma z[(z^2 + c^2)^{\sigma-1} - (z^2 + d^2)^{\sigma-1}]$$

Note that $(z^2 + c^2)^{\sigma-1} > (z^2 + d^2)^{\sigma-1}$ for $\sigma \in (0, 1)$. So, $\gamma'_{c,d}(z) > 0$. Thus, $\gamma_{c,d}(z)$ is a strictly increasing function.

This concludes the proof. □

Lemma 4.1.2. *Let z and σ are real numbers, where $z \geq 1$ and $\sigma \in (0, 1)$. Then*

(i) $\Gamma_0(z) = (12z + 8)^\sigma - (3z + 2)^\sigma$ *is strictly increasing.*

(ii) $\Gamma_1(z) = (15z + 2)^\sigma - (15z - 5)^\sigma$ *is strictly decreasing.*

(iii) $\Gamma_2(z) = (8z + 9)^\sigma - (8z + 2)^\sigma$ *is strictly decreasing.*

(iv) $\Gamma_3(z) = (3z + 14)^\sigma - (3z + 2)^\sigma$ *is strictly decreasing.*

(v) $\Gamma_4(z) = (12z+8)^\sigma - (12z-7)^\sigma$ *is strictly decreasing.*

Proof. (i). We obtain

$$\Gamma_0'(z) = 3\sigma[4(12z+8)^{\sigma-1} - (3z+2)^{\sigma-1}].$$

Consider the function $\Psi(\sigma) = 4(\frac{12z+8}{3z+2})^{\sigma-1}$, where $z \geq 1$ and $\sigma \in (0,1)$. It can be easily verified that $\Psi''(\sigma) > 0$. This implies that $\Psi(\sigma)$ is strictly convex. We get $\Psi(1) > 1$ and $\Psi(0) = 1$. So, $\Psi(\sigma) > 1$ for $\sigma \in (0,1)$. This holds $4(12z+8)^{\sigma-1} > (3z+2)^{\sigma-1}$ for $\sigma \in (0,1)$. It means that $\Gamma_0'(z) > 0$. Hence $\Gamma_0(z)$ is a strictly increasing function for $\sigma \in (0,1)$.
(ii). We obtain

$$\Gamma_1'(z) = 15\sigma[(15z+2)^{\sigma-1} - (15z-5)^{\sigma-1}].$$

Since $\sigma \in (0,1)$, it follows that $(15z+2)^{\sigma-1} < (15z-5)^{\sigma-1}$. So, $\Gamma_1'(z) < 0$, implies that $\Gamma_1(z)$ is strictly decreasing. The proofs of $(iii), (iv)$ and (v) follow in a similar manner to that of (ii). □

Lemma 4.1.3. *For* $\sigma \in (0,1)$*, we have*

(i) $2(25)^\sigma - 32^\sigma - 18^\sigma > 0$,

(ii) $2(20)^\sigma - 5^\sigma - 32^\sigma > 0$.

Proof. By Lemma 3.1.2, the functions

$$\Lambda_{\frac{32}{25},\frac{18}{25}}(\sigma) = (\frac{32}{25})^\sigma + (\frac{18}{25})^\sigma \text{ and } \Lambda_{\frac{5}{20},\frac{32}{20}}(\sigma) = (\frac{5}{20})^\sigma + (\frac{32}{20})^\sigma$$

are strictly convex for real number σ. We have

$$\Lambda_{\frac{32}{25},\frac{18}{25}}(0) = 2 = \Lambda_{\frac{32}{25},\frac{18}{25}}(1) \text{ and } \Lambda_{\frac{5}{20},\frac{32}{20}}(0) = 2 = \Lambda_{\frac{5}{20},\frac{32}{20}}(1).$$

(i). We obtain $\Lambda_{\frac{32}{25},\frac{18}{25}}(\sigma) < 2$ for $\sigma \in (0,1)$. This implies $32^\sigma + 18^\sigma < 2(25)^\sigma$ for $\sigma \in (0,1)$.

(ii). We obtain $\Lambda_{\frac{32}{20},\frac{5}{20}}(\sigma) < 2$ for $\sigma \in (0,1)$. This implies $32^\sigma + 5^\sigma < 2(20)^\sigma$ for $\sigma \in (0,1)$. $\square$

4.2 Chemical trees in $\mathbb{CT}(n,b)$ with maximum $\mathbb{SO}_\sigma$ index for $\sigma \in (0,1)$

In this section, we will determine the maximum general Sombor index's chemical trees in $\mathbb{CT}(n,b)$. We further classify $\mathbb{CT}(n,b)$ into two classes for finding the maximum general Sombor index in $\mathbb{CT}(n,b)$ given in Section 3.2. Now, we need the following lemma to prove the main theorem:

Lemma 4.2.1. *Let $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n,b)$ be a chemical tree of order $2b+2 \le n \le 3b+2$ and $b \ge 1$ with maximum $\mathbb{SO}_\sigma$ index for $\sigma \in (0,1)$. Then*

(i) $n_2(T_1) = 0$,

(ii) $n_3(T_1) = 3b+2-n$, $n_1(T_1) = n-b$ and $n_4(T_1) = n-2b-2$.

Proof. (i) Contrarily, $n_2(T_1) \ge 1$. Then there occurs $w \in V(T_1)$ so that $d_{T_1}(w) = 2$. Assume $N_{T_1}(w) = \{w_1, w_2\}$. We claim that $n_3(T_1) \ge 1$. For if $n_3(T_1) = 0$, then by solving (3.2) and (3.3) simultaneously, we note that $n_1(T_1) = 2 + 2n_4(T_1)$. Now, from (3.2), we note that $n \ge 3b+3$, which is a contradiction because $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n,b)$ has $n \le 3b+2$. Thus, there occurs a vertex $x \in V(T_1)$ so that $d_{T_1}(x) = 3$. Assume $N_{T_1}(x) = \{x_1, x_2, x_3\}$. To avoid complexity, assume that x_1 and w_1 lie on x,w-path in T_1 (w_1 and x_1 may coincide with each other). Thus, we have $2 \le d_{T_1}(x_1) \le 4$, $2 \le d_{T_1}(w_1) \le 4$, $1 \le d_{T_1}(x_2) \le 4$, $1 \le d_{T_1}(x_3) \le 4$ and $1 \le d_{T_1}(w_2) \le 4$. Now, we get $T_2 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n,b)$ from T_1 as:

$$T_2 = T_1 - ww_2 + xw_2.$$

This implies $d_{T_2}(x) = d_{T_1}(x) + 1 = 4$, $d_{T_2}(w) = d_{T_1}(w) - 1 = 1$ and $d_{T_2}(u) = d_{T_1}(u)$ for all $u \in V(T_1) \setminus \{x, w\}$. Now we discuss the proof in two cases.

Case 1. If $wx \notin E(T_1)$, then to show $\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > 0$, we note that

$$\begin{aligned}\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) = &\sum_{i=2}^{3}\Big((4^2 + d_{T_1}(x_i)^2)^\sigma - (3^2 + d_{T_1}(x_i)^2)^\sigma\Big)\\ &+ (4^2 + d_{T_1}(x_1)^2)^\sigma - (3^2 + d_{T_1}(x_1)^2)^\sigma\\ &+ (4^2 + d_{T_1}(w_2)^2)^\sigma - (2^2 + d_{T_1}(w_2)^2)^\sigma\\ &+ (1^2 + d_{T_1}(w_1)^2)^\sigma - (2^2 + d_{T_1}(w_1)^2)^\sigma.\end{aligned}$$

Since $\sigma > 0$, it follows that

$$\begin{aligned}\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > &(4^2 + d_{T_1}(w_2)^2)^\sigma - (2^2 + d_{T_1}(w_2)^2)^\sigma\\ &+ (1^2 + d_{T_1}(w_1)^2)^\sigma - (2^2 + d_{T_1}(w_1)^2)^\sigma.\end{aligned}$$

By using Lemma 4.1.1 (i) and (ii), we obtain

$$\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > (32)^\sigma - (20)^\sigma + 5^\sigma - 8^\sigma.$$

Since by Lemma 4.1.2 (i), we have $(20)^\sigma - 5^\sigma < (32)^\sigma - 8^\sigma$. So, $\mathbb{SO}_\sigma(T_2) > \mathbb{SO}_\sigma(T_1)$, leads to a contradiction.

Case 2. If $wx \in E(T_1)$, then to show $\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > 0$, we note that

$$\begin{aligned}\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) = &\sum_{i=2}^{3}\Big((4^2 + d_{T_1}(x_i)^2)^\sigma - (3^2 + d_{T_1}(x_i)^2)^\sigma\Big)\\ &+ (4^2 + d_{T_1}(w_2)^2)^\sigma - (2^2 + d_{T_1}(w_2)^2)^\sigma.\end{aligned}$$

Since $\sigma > 0$, it follows that $\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > 0$. A contradiction arises from each case. Therefore, $n_2(T_1) = 0$.

(ii) By using Lemma 4.2.1 (i) in (3.2) and (3.3) and solving them simultaneously, we note that

$$n_1(T_1) = n - b,$$
$$n_3(T_1) = 3b + 2 - n,$$
$$n_4(T_1) = n - 2b - 2.$$

This concludes the proof. □

Lemma 4.2.2. *Let $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ be a chemical tree of order $2b + 2 \leq n \leq \left\lfloor \frac{5b+5}{2} \right\rfloor$ and $b \geq 2$ with maximum $\mathbb{SO}_\sigma$ index for $\sigma \in (0, 1)$. Then*

(i) $m_{12}(T_1) = m_{22}(T_1) = m_{23}(T_1) = m_{24}(T_1) = 0$,

(ii) $m_{44}(T_1) = 0$,

(iii) $m_{14}(T_1) = 3n_4(T_1)$,

(iv) $m_{13}(T_1) = 5b - 2n + 6$, $\quad m_{34}(T_1) = n_4(T_1)$ *and* $m_{33}(T_1) = 3b - n + 1$.

Proof. *(i)* The proof follows instantly from Lemma 4.2.1 *(i)*.

(ii) Contrarily, $m_{44}(T_1) \geq 1$. Then $xy \in E(T_1)$ so that $d_{T_1}(x) = 4 = d_{T_1}(y)$. We further claim that $m_{13}(T_1)$ and $m_{33}(T_1)$ can not be zero simultaneously. For if $m_{13}(T_1) = 0 = m_{33}(T_1)$, then by using Lemmas 4.2.1, 4.2.2 *(i)* in (3.4), we note that $m_{14}(T_1) = n - b$ and $m_{34}(T_1) = 9b + 6 - 3n$. Now, by substituting the values of $m_{14}(T_1), m_{34}(T_1)$ and Lemma 4.2.1 *(ii)* in (3.4), it follows that $m_{44}(T_1) = 3n - 8b - 7$. Since $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ has $n \leq \left\lfloor \frac{5b+5}{2} \right\rfloor$, which implies $m_{44}(T_1) \leq \frac{1-b}{2} < 0$, which is a contradiction. Hence, $m_{13}(T_1)$ and $m_{33}(T_1)$ cannot be zero simultaneously. Now, we further discuss the proof in two cases:

Case 1. If $m_{13}(T_1) \geq 1$, Then $uv \in E(T_1)$ so that $d_{T_1}(u) = 1$ and $d_{T_1}(v) = 3$. To avoid complexity, assume that x lies on u, y-path in T_1. Now, we get $T_2 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ from T_1 as:

$$T_2 = T_1 - xy - uv + vy + ux. \tag{4.2}$$

This implies $d_{T_2}(w) = d_{T_1}(w)$ for all $w \in V(T_1)$. Then to show $\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > 0$, we note that

$$\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > (17)^\sigma - (32)^\sigma + (25)^\sigma - (10)^\sigma.$$

Since by Lemma 4.1.2 (ii), we have $\Gamma_1(1) = (17)^\sigma - (10)^\sigma > (32)^\sigma - (25)^\sigma = \Gamma_1(2)$. So, $\mathbb{SO}_\sigma(T_2) > \mathbb{SO}_\sigma(T_1)$, leads to a contradiction.

Case 2. If $m_{33}(T_1) \geq 1$, Then $uv \in E(T_1)$ so that $d_{T_1}(u) = 3 = d_{T_1}(v)$. To avoid complexity, assume that x and v lie on u, y-path in T_1. To show $\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > 0$, we perform the following calculation using the transformation (4.2):

$$\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > 2(25)^\sigma - (32)^\sigma - (18)^\sigma > 0.$$

By Lemma 4.1.3 (i), this leads to a contradiction. A contradiction arises from each case, implying $m_{44}(T_1) = 0$.

(iii) Contrarily, $m_{14}(T_1) \neq 3n_4(T_1)$. Now, we discuss the proof in two cases:

Case 1. If $m_{14}(T_1) > 3n_4(T_1)$, we obtain a disconnected tree.

Case 2. Assume that $m_{14}(T_1) < 3n_4(T_1)$, implying that there occurs a vertex of degree 4 with at least two non-pendent neighbors. Let $w \in V(T_1)$ be a vertex of degree 4 with at least two non-pendent neighbors say, w_1 and w_2. From Lemma 4.2.1 (i), it is clear that $3 \leq d_{T_1}(w_1) \leq 4$, and $3 \leq d_{T_1}(w_2) \leq 4$. We further claim that if $m_{14}(T_1) < 3n_4(T_1)$, then $m_{13}(T_1) \geq 1$. For if $m_{13}(T_1) = 0$, then from Lemmas 4.2.1 and 4.2.2 (i) in (3.4), we derive $m_{14}(T_1) = n - b$ or $n - b < 3n - 6b - 6$, implying $n > \frac{5b+6}{2}$. Since $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ has $n \leq \left\lfloor \frac{5b+5}{2} \right\rfloor$, which implies a contradiction. Thus, there occurs $uv \in E(T_1)$ so that $d_{T_1}(u) = 3$ and $d_{T_1}(v) = 1$. To avoid complexity, assume that w_2 lies on w, u-path (w_2

may coincide with u). Now, we get $T_2 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n,b)$ from T_1 as:

$$T_2 = T_1 - ww_1 - uv + wv + uw_1.$$

This implies $d_{T_2}(t) = d_{T_1}(t)$ for all $t \in V(T_1)$. Then to give demonstration of $\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > 0$, we note that

$$\begin{aligned}\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) = (1^2+4^2)^\sigma - (3^2+1^2)^\sigma + (3^2 + d_{T_1}(w_1)^2)^\sigma \\ - (4^2 + d_{T_1}(w_1)^2)^\sigma.\end{aligned}$$

By using Lemma 4.1.1 (*ii*), we obtain

$$\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > (17)^\sigma - (10)^\sigma + (18)^\sigma - (25)^\sigma > 0.$$

Since by Lemma 4.1.2 (iii), we have $\Gamma_2(1) = (17)^\sigma - (10)^\sigma > (25)^\sigma - (18)^\sigma = \Gamma_2(2)$. So, $\mathbb{SO}_\sigma(T_2) > \mathbb{SO}_\sigma(T_1)$, leads to a contradiction. This results in a contradiction. Therefore, $m_{14}(T_1) = 3n_4(T_1)$.

(*iv*) By using Lemma 4.2.2 (*i*) – (*iii*) in (3.4), we note that

$$\begin{aligned} m_{13}(T_1) &= 5b - 2n + 6, \\ m_{34}(T_1) &= n_4(T_1), \\ m_{33}(T_1) &= 3b - n + 1. \end{aligned}$$

This concludes the proof. □

Lemma 4.2.3. *Let $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n,b)$ be a chemical tree of order $\left\lceil \frac{5b+6}{2} \right\rceil \le n \le \left\lfloor \frac{8b+7}{3} \right\rfloor$ and $b \ge 6$ with maximum $\mathbb{SO}_\sigma$ index for $\sigma \in (0,1)$. Then*

(*i*) $m_{12}(T_1) = m_{22}(T_1) = m_{23}(T_1) = m_{24}(T_1) = 0$,

(*ii*) $m_{13}(T_1) = 0$,

(*iii*) $m_{14}(T_1) = n - b$,

(*iv*) $m_{44}(T_1) = 0$,

(*v*) $m_{34}(T_1) = 3n - 7b - 8$ *and* $m_{33}(T_1) = 8b + 7 - 3n$.

Proof. (*i*) The proof follows instantly from Lemma 4.2.1 (*i*).

(*ii*) Contrarily, $m_{13}(T_1) \geq 1$. Then $uv \in E(T_1)$ so that $d_{T_1}(v) = 1$ and $d_{T_1}(u) = 3$. Further, we claim that $m_{14}(T_1) < 3n - 6b - 6$. For if $m_{14}(T_1) = 3n - 6b - 6$, then by using Lemma 4.2.3 (*i*) in (3.4), we note that $m_{13}(T_1) = 5b - 2n + 6$. Since $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ has $n \geq \left\lceil \frac{5b+6}{2} \right\rceil$, implying $m_{13}(T_1) \leq 5b - 2\left\lceil \frac{5b+6}{2} \right\rceil + 6 \leq 0$. This gives a contradiction. Thus $m_{14}(T_1) < 3n - 6b - 6$. Now, we suppose that w is a vertex of degree 4 with at least two non-pendant neighbors, say w_2 and w_1. From Lemma 4.2.1, it is clear that $3 \leq d_{T_1}(w_1) \leq 4$ and $3 \leq d_{T_1}(w_2) \leq 4$. To avoid complexity, assume that w_2 lies on w, u-path (w_2 and u may coincide). Now, by following transformation and calculations of Lemma 4.2.2 (*iii*), it follows that $m_{13}(T_1) = 0$.

(*iii*) By substituting Lemma 4.2.3 (*i*)$-$(*ii*) in (3.4), we note that $m_{14}(T_1) = n_1(T_1)$.

(*iv*) Contrarily, let $m_{44}(T_1) \geq 1$. Then $xy \in E(T_1)$ so that $d_{T_1}(x) = 4 = d_{T_1}(y)$. Further, we claim that $m_{33}(T_1) \geq 1$. On the contrary, let $m_{33}(T_1) = 0$. Then from Lemmas 4.2.3 (*i*)$-$(*iii*) and (3.4), we note that $m_{34}(T_1) = 9b + 6 - 3n$. From Lemmas 4.2.1, 4.2.3 (*iii*) and $m_{34}(T_1) = 9b + 6 - 3n$, we derive $m_{44}(T_1) = 3n - 8b - 7$. Since $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ has $n \leq \left\lfloor \frac{8b+7}{3} \right\rfloor$, it follows that $m_{44}(T_1) \leq 3\left\lfloor \frac{8b+7}{3} \right\rfloor - 8b - 7 \leq 0$, which is a contradiction. Thus, there occurs $uv \in E(T_1)$ so that $d_{T_1}(u) = 3 = d_{T_1}(v)$. To avoid complexity, assume that x and v lie on u, y-path. Now, by following the transformation and calculations from Case 2 of Lemma 4.2.2 (*ii*), we note that $m_{44}(T_1) = 0$.

(*v*) By substituting Lemma 4.2.1 and 4.2.3 $(i)-(iv)$ in (3.4), we note that

$$m_{34}(T_1) = 3n - 7b - 8,$$
$$m_{33}(T_1) = 8b + 7 - 3n.$$

This concludes the proof. $\square$

Lemma 4.2.4. *Let $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n,b)$ be a chemical tree of order $\lceil \frac{8b+8}{3} \rceil \leq n \leq 3b+2$ and $b \geq 2$ with maximum $\mathbb{SO}_\sigma$ index for $\sigma \in (0,1)$. Then*

(*i*) $m_{12}(T_1) = m_{22}(T_1) = m_{23}(T_1) = m_{24}(T_1) = 0,$

(*ii*) $m_{13}(T_1) = 0,$

(*iii*) $m_{14}(T_1) = n_1(T_1),$

(*iv*) $m_{33}(T_1) = 0,$

(*v*) $m_{34}(T_1) = 3n_3(T_1)$ *and* $m_{44}(T_1) = 3n - 8b - 7.$

Proof. (*i*) The proof follows instantly from Lemma 4.2.1 (*i*).

(*ii*) Contrarily, let $m_{13}(T_1) \geq 1$. Then $uv \in E(T_1)$ so that $d_{T_1}(v) = 1$ and $d_{T_1}(u) = 3$. Further, we claim that $m_{14}(T_1) < 3n - 6b - 6$. By contradiction, assume that $m_{14}(T_1) = 3n-6b-6$, then by using Lemma 4.2.4 (*i*) in (3.4), we note that $m_{13}(T_1) = 5b - 2n + 6$. Since $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n,b)$ has $n \geq \lceil \frac{8b+8}{3} \rceil$, implying $m_{13}(T_1) \leq \frac{-b+2}{3} \leq 0$, when $b \geq 2$. This gives a contradiction. Thus $m_{14}(T_1) < 3n-6b-6$. The remaining proof is similar to the proof of Lemma 4.2.3 (*ii*). Hence, $m_{13} = 0$.

(*iii*) The proof is similar to proof of Lemma 4.2.3 (*iii*).

(*iv*) Contrarily, let $m_{33}(T_1) \geq 1$. Then $uv \in E(T_1)$ so that $d_{T_1}(u) = 3 = d_{T_1}(v)$. Further, we claim that $m_{44}(T_1) \neq 0$. By contradiction, assume that $m_{44}(T_1) = 0$. By using Lemmas 4.2.1 and 4.2.4 $(i)-(iii)$ in (3.4), we note that $m_{34}(T_1) = 3n - 7b - 8$. Then from Lemma 4.2.4 $(i) - (ii)$ and $m_{34}(T_1) = 3n - 7b - 8$, it follows that $m_{33}(T_1) = 8b + 7 - 3n$. Since $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ has $n \geq \left\lceil \frac{8b+8}{3} \right\rceil$, we get $m_{33}(T_1) \leq 8b + 7 - 3\left\lceil \frac{8b+8}{3} \right\rceil \leq 0$, which is a contradiction. Thus, there occurs $xy \in E(T_1)$ so that $d_{T_1}(x) = 4 = d_{T_1}(y)$. For simplicity, assume that x and v lie on u, y-path. Now, by following the transformation and calculations of Case 2 of Lemma 4.2.2 (ii), we note that $m_{33}(T_1) = 0$

(v) By using Lemmas 4.2.1, 4.2.4 $(i) - (iv)$ in (3.4), we note that

$$m_{34}(T_1) = 9b + 6 - 3n,$$
$$m_{44}(T_1) = 3n - 8b - 7.$$

This concludes the proof. □

Lemma 4.2.5. *Let $T_1 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ be a chemical tree of order 13 and $b = 4$ with maximum $\mathbb{SO}_\sigma$ index for $\sigma \in (0, 1)$. Then*

(i) $m_{12}(T_1) = m_{22}(T_1) = m_{23}(T_1) = m_{24}(T_1) = 0$,

(ii) $n_1(T_1) = 9$, $n_3(T_1) = 1$, $n_4(T_1) = 3$,

(iii) $m_{33}(T_1) = 0$,

(iv) $m_{44}(T_1) = 0$,

(v) $m_{13}(T_1) = 0$, $m_{14}(T_1) = 9$ *and* $m_{34}(T_1) = 3$.

Proof. (i) The proof is direct outcome of Lemma 4.2.1 (i).

(ii) The proof is direct outcome of Lemma 4.2.1 (ii).

(iii) The proof is the direct outcome of Lemma 4.2.5 (ii).

(iv) Contrarily, let $m_{44}(T_1) \geq 1$. Then $xy \in E(T_1)$ so that $d_{T_1}(x) = 4 = d_{T_1}(y)$. We claim that $m_{13}(T_1) \neq 0$. Let $m_{13}(T_1) = 0$. Then by using

Lemma 4.2.5 $(i)-(iii)$ in (3.4), we get $m_{14}(T_1) = 9$ and $m_{34}(T_1) = 3$. Now, using $m_{14}(T_1) = 9$ and $m_{34}(T_1) = 3$ in (3.4), we get $m_{44}(T_1) = 0$. Since $m_{44}(T_1) \geq 1$, we note that a contradiction. Hence, then there occurs $uv \in E(T_1)$ so that $d_{T_1}(u) = 1$ and $d_{T_1}(v) = 3$. To avoid complexity, assume that x lies on u, y-path in T_1. Now, by following the transformation and calculations from Case 1 of Lemma 4.2.2 (i), we note that $m_{44}(T_1) = 0$.

(v) By substituting Lemmas 4.2.5 $(i)-(iv)$ in (3.4), we note that

$$m_{13}(T_1) = 0,$$
$$m_{14}(T_1) = 9,$$
$$m_{34}(T_1) = 3.$$

This concludes the proof. □

Lemma 4.2.6. *Let $T_1 \in \mathbb{C}_2\mathbb{T}(n, b)$ be a chemical tree of order $n \geq 3b + 3$ and $b \geq 1$ with maximum $\mathbb{SO}_\sigma$ index for $\sigma \in (0, 1)$. Then*

(i) $n_3(T_1) = 0$,

(ii) $n_1(T_1) = 2b + 2$, $\quad n_2(T_1) = n - 3b - 2$ *and* $n_4(T_1) = b$.

Proof. (i) Contrarily, let $n_3(T_1) \geq 1$. Then there occurs $x \in V(T_1)$ so that $d_{T_1}(x) = 3$. Assume $N_{T_1}(x) = \{x_1, x_2, x_3\}$. Further, we claim that $n_2(T_1) \geq 1$. On the contrary, let $n_2(T_1) = 0$. Then from (3.2) and (3.3) we note that $n = 2+2b+n_4(T_1)$. Now, if $n_4(T_1) = 0$, we get $n = 2b+2$ and if $n_4(T_1) \leq b$, we note that $n \leq 3b + 2$. In either case, we get a contradiction because $T_1 \in \mathbb{C}_2\mathbb{T}(n, b)$ has $n \geq 3b+3$. Thus, there occurs a vertex $w \in V(T_1)$ so that $d_{T_1}(w) = 2$. Assume $N_{T_1}(w) = \{w_1, w_2\}$. To avoid complexity, assume that x_1 and w_1 lie on x, w-path (w_1 and x_1 may coincide). This implies that $2 \leq d_{T_1}(x_1) \leq 4$, $2 \leq d_{T_1}(w_1) \leq 4$, $1 \leq d_{T_1}(x_2) \leq 4$, $1 \leq d_{T_1}(x_3) \leq 4$ and $1 \leq d_{T_1}(w_2) \leq 4$. Now, by following the transformation and calculations from Lemma 4.2.1 (i), we note that $n_3(T_1) = 0$.

(ii) By using Lemma 4.2.6 (i) in (3.2) and (3.3), then by solving them simultaneously, we note that

$$n_1(T_1) = 2b + 2,$$
$$n_2(T_1) = n - 3b - 2,$$
$$n_4(T_1) = b.$$

This concludes the proof. □

Lemma 4.2.7. *Let $T_1 \in \mathbb{C}_2\mathbb{T}(n, b)$ be a chemical tree of order $n \geq 3b + 3$ and $b = 1$ with maximum $\mathbb{SO}_\sigma$ index for $\sigma \in (0, 1)$. Then*

(i) $m_{13}(T_1) = m_{23}(T_1) = m_{33}(T_1) = m_{34}(T_1) = 0$,

(ii) $n_1(T_1) = 4$, $n_2(T_1) = n - 5$, $n_4(T_1) = 1$,

(iii) $m_{44}(T_1) = 0$

(iv) $m_{14}(T_1) = 3$,

(v) $m_{22}(T_1) = n - 6$, $m_{12}(T_1) = 1$ *and* $m_{24}(T_1) = 1$.

Proof. (i) The proof follows instantly from Lemma 4.2.6 (i).

(ii) By using $b = 1$ in Lemma 4.2.6 (ii), we note that $n_1(T_1) = 4$, $n_2(T_1) = n - 5$ and $n_4(T_1) = 1$.

(iii) This is an immediate outcome of Lemma 4.2.7 (ii).

(iv) Contrarily, let $m_{14}(T_1) \neq 3$. We discuss this in two cases.
Case 1. If $m_{14}(T_1) = 4$, the tree become disconnected.
Case 2. Let $m_{14}(T_1) < 3$. Then there occurs$w \in V(T_1)$ with degree 4. Assume $N_{T_1}(w) = \{w_1, w_2, w_3, w_4\}$. Since $m_{14}(T_1) < 3$, it follows

that w has at least two non-pendent neighbors. To avoid complexity, we assume that w_1 and w_2 are non-pendent neighbors of w. Let $x \notin N_{T_1}(w)$ be a pendent vertex, and x_1 be its neighbor. To avoid complexity, assume that w_2 lies on w, x-path (w_2 may coincide with x_1). Since $b = 1$, it implies $d_{T_1}(w_1) = 2 = d_{T_1}(w_2)$, and $d_{T_1}(x_1) = 2$. Now, we get $T_2 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ from T_1 as:

$$T_2 = T_1 - ww_1 - xx_1 + wx + x_1w_1$$

This implies $d_{T_2}(t) = d_{T_1}(t)$ for all $t \in V(T_1)$. Then to show $\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > 0$, we note that

$$\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) = 17^\sigma - 20^\sigma + 8^\sigma - 5^\sigma.$$

Since by Lemma 4.1.2 (iv), $\Gamma_3(1) = 17^\sigma - 5^\sigma > 20^\sigma - 8^\sigma = \Gamma_3(2)$. So, $\mathbb{SO}_\sigma(T_2) > \mathbb{SO}_\sigma(T_1)$, which leads to a contradiction. Therefore, $m_{14}(T_1) = 3$.

(v) By using Lemma 4.2.7 $(i) - (iv)$ in (3.4), we note that

$$\begin{aligned} m_{22}(T_1) &= n - 6, \\ m_{12}(T_1) &= 1, \\ m_{24}(T_1) &= 1. \end{aligned}$$

This concludes the proof. □

Lemma 4.2.8. *Let $T_1 \in \mathbb{C}_2\mathbb{T}(n, b)$ be a chemical tree of order $3b + 3 \le n \le 4b + 1$ and $b \ge 2$ with maximum $\mathbb{SO}_\sigma$ index for $\sigma \in (0, 1)$. Then*

(i) $m_{13}(T_1) = m_{23}(T_1) = m_{33}(T_1) = m_{34}(T_1) = 0,$

(ii) $m_{12}(T_1) = 0,$

(iii) $m_{14}(T_1) = n_1(T_1)$

(*iv*) $m_{22}(T_1) = 0$,

(*v*) $m_{44}(T_1) = 4b + 1 - n$ *and* $m_{24}(T_1) = 2n - 6b - 4$.

Proof. (*i*) The proof follows instantly from Lemma 4.2.6 (*i*).

(*ii*) Contrarily, let $m_{12}(T_1) \geq 1$. Then $xx_1 \in E(T_1)$ so that $d_{T_1}(x_1) = 2$ and $d_{T_1}(x) = 1$. Since $b \geq 2$, it follows that T_1 has at least two branching vertices. Therefore, suppose that $v, w \in V(T_1)$ so that $d_{T_1}(w) = 4 = d_{T_1}(v)$. To avoid complexity, suppose that w lies on the x, v-path. Now, we discuss the proof in two cases:

Case 1. When $vw \in E(T_1)$. Then we get $T_2 \in \mathbb{C}_2\mathbb{T}(n, b)$ from T_1 as:

$$T_2 = T_1 - xx_1 - vw + vx_1 + wx.$$

This implies $d_{T_2}(u) = d_{T_1}(u)$ for all $u \in V(T_1)$. Then to show $\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > 0$, we note that

$$\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) = 20^\sigma - 5^\sigma + 17^\sigma - 32^\sigma.$$

Since by Lemma 4.1.2 (v), $\Gamma_4(1) = 20^\sigma - 5^\sigma > (32)^\sigma - (17)^\sigma = \Gamma_4(2)$. So, $\mathbb{SO}_\sigma(T_2) > \mathbb{SO}_\sigma(T_1)$, which leads to a contradiction.

Case 2. When $vw \notin E(T_1)$. Then v and w are connected by shortest path $P_{vw} = vw_s \cdots w_1 w$ and $d_{T_1}(w_s) = 2$, where $s \geq 1$. Now, we get $T_2 \in \mathbb{C}_2\mathbb{T}(n, b)$ from T_1 as:

$$T_2 = T_1 - ww_1 - xx_1 + wx + x_1 w_1.$$

This implies $d_{T_2}(t) = d_{T_1}(t)$ for all $t \in V(T_1)$. Now, the calculations are similar to Lemma 4.2.7 (*iv*), implying $m_{12}(T_1) = 0$.

(*iii*) By using Lemma 4.2.8 (*i*) – (*ii*) in (3.4), we get $m_{14}(T_1) = n_1(T_1)$.

(*iv*) Contrarily, assume that $m_{22}(T_1) \neq 0$. Then $xy \in E(T_1)$ so that

$d_{T_1}(x) = 2 = d_{T_1}(y)$. We further claim that if $m_{22}(T_1) \geq 1$, then $m_{44}(T_1) \geq 1$. For if $m_{44}(T_1) = 0$. Then by using Lemmas 4.2.8 $(i)-(iii)$ in (3.4) we get $m_{24}(T_1) = 2b - 2$. From Lemmas 4.2.6, 4.2.8 $(i) - (ii)$ and $m_{24}(T_1) = 2b - 2$, we note that $m_{22}(T_1) = n - 4b - 1$. Since $T_1 \in \mathbb{C}_2\mathbb{T}(n, b)$ has $n \leq 4b + 1$, it follows that $m_{22}(T_1) \leq 0$. This contradicts the supposition. Thus, there occurs $uv \in E(T_1)$ so that $d_{T_1}(u) = 4 = d_{T_1}(v)$. To avoid complexity, assume that x and v lie on the y, u-path. Now, we get $T_2 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ from T_1 as:

$$T_2 = T_1 - uv - xy + ux + yv.$$

This implies $d_{T_2}(t) = d_{T_1}(t)$ for all $t \in V(T_1)$. Then to show $\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) > 0$, we note that

$$\mathbb{SO}_\sigma(T_2) - \mathbb{SO}_\sigma(T_1) = 2(20)^\sigma - (32)^\sigma - 8^\sigma.$$

Since by Lemma 4.1.3 (ii), contradiction holds. Therefore, $m_{22}(T_1) = 0$.

(v) By using Lemma 4.2.8 $(i) - (iv)$ in (3.4), we get

$$m_{44}(T_1) = 4b + 1 - n,$$
$$m_{24}(T_1) = 2n - 6b - 4.$$

This concludes the proof. □

Lemma 4.2.9. *Let $T_1 \in \mathbb{C}_2\mathbb{T}(n, b)$ be a chemical tree of order $n \geq 4b + 2$ and $b \geq 2$ with maximum $\mathbb{SO}_\sigma$ index for $\sigma \in (0, 1)$. Then*

(i) $m_{13}(T_1) = m_{23}(T_1) = m_{33}(T_1) = m_{34}(T_1) = 0$,

(ii) $m_{12}(T_1) = 0$,

(iii) $m_{14}(T_1) = 2b + 2$.

(iv) $m_{44}(T_1) = 0$,

(v) $m_{22}(T_1) = n - 4b - 1$ *and* $m_{24}(T_1) = 2b - 2$.

Proof. (i) The proof follows instantly from Lemma 4.2.6 (i).

(ii) The proof is similar to the proof of Lemma 4.2.8 (ii).

(iii) The proof is similar to the proof of Lemma 4.2.8 (iii).

(iv) Contrarily, let $m_{44}(T_1) \geq 1$. Then $xy \in E(T_1)$ so that $d_{T_1}(x) = 4 = d_{T_1}(y)$. We further claim that if $m_{44}(T_1) \geq 1$, then $m_{22}(T_1) \geq 1$. For if $m_{22}(T_1) = 0$, then by using Lemmas 4.2.6 and 4.2.9 (i) − (ii) in (3.4), we get $m_{24}(T_1) = 2n - 6b - 4$. From Lemmas 4.2.6, 4.2.9 (i) − (iii) and $m_{24}(T_1) = 2n - 6b - 4$, it follows that $m_{44}(T_1) = 4b + 1 - n$. Since $T_1 \in \mathbb{C}_2\mathbb{T}(n, b)$ has order $n \geq 4b + 2$, it follows that $m_{44}(T_1) < 0$. This contradicts the supposition. Therefore, there occurs $xy \in E(T_1)$ so that $d_{T_1}(x) = 2 = d_{T_1}(y)$. To avoid complexity assume that x and v lie on y, u-path. Now, we get $T_2 \in \mathbb{C}_{\mathbb{1}}\mathbb{T}(n, b)$ from T_1 as:

$$T_2 = T_1 - uv - xy + ux + yv$$

This implies $d_{T_2}(t) = d_{T_1}(t)$ for all $t \in V(T_1)$. By following the transformation and calculations from Lemma 4.2.8 (iv), we note that $m_{44}(T_1) = 0$.

(v) By using Lemma 4.2.9 (i) − (iv) in (3.4), we get

$$m_{22}(T_1) = n - 4b - 1,$$
$$m_{24}(T_1) = 2b - 2.$$

This conclude the proof. □

Theorem 4.2.1. *Let* $\mathbb{C}\mathbb{T}(n, b)$ *be a chemical tree of order* $n \geq 2b + 2$ *and*

$b \geq 1$ *with maximum* $\mathbb{SO}_\sigma$ *index for* $\sigma \in (0,1)$. *Then*

$$\mathbb{SO}_\sigma(T_1) = \begin{cases} 3(10)^\sigma, & \text{if } n = 4 \text{ and } b = 1; \\ 4(17)^\sigma, & \text{if } n = 5 \text{ and } b = 1; \\ 9(17)^\sigma + 3(25)^\sigma, & \text{if } n = 13 \text{ and } b = 4; \\ n(3(17)^\sigma - 2(10)^\sigma + (25)^\sigma - (18)^\sigma) + b(-6(17)^\sigma + 5(10)^\sigma \\ -2(25)^\sigma + 3(18)^\sigma) - 6(17)^\sigma + 6(10)^\sigma - 2(25)^\sigma \\ +(18)^\sigma, & \text{if } 2b+2 \leq n \leq \lfloor \frac{5b+5}{2} \rfloor \text{ and } b \geq 2; \\ n((17)^\sigma + 3(25)^\sigma - 3(18)^\sigma) + b(-(17)^\sigma - 7(25)^\sigma + 8(18)^\sigma) \\ -8(25)^\sigma + 7(18)^\sigma, & \text{if } \lceil \frac{5b+6}{2} \rceil \leq n \leq \lfloor \frac{8b+7}{3} \rfloor \text{ and } b \geq 6; \\ n((17)^\sigma - 3(25)^\sigma + 3(32)^\sigma) + b(-(17)^\sigma + 9(25)^\sigma - 8(32)^\sigma) \\ +6(25)^\sigma - 7(32)^\sigma, & \text{if } \lceil \frac{8b+8}{3} \rceil \leq n \leq 3b+2 \text{ and } b \geq 2; \\ n(8)^\sigma + 3(17)^\sigma + (20)^\sigma + (5)^\sigma \\ -6(8)^\sigma, & \text{if } n \geq 3b+3 \text{ and } b = 1; \\ n(-(32)^\sigma + 2(20)^\sigma) + b(2(17)^\sigma + 4(32)^\sigma - 6(20)^\sigma) + 2(17)^\sigma \\ +(32)^\sigma - 4(20)^\sigma, & \text{if } 3b+3 \leq n \leq 4b+1 \text{ and } b \geq 2; \\ n(8)^\sigma + b(2(17)^\sigma - 4(8)^\sigma + 2(20)^\sigma) + 2(17)^\sigma \\ -(8)^\sigma - 2(20)^\sigma, & \text{if } n \geq 4b+2 \text{ and } b \geq 2. \end{cases}$$

Proof. **Case 1.** When $n = 4$ and $b = 1$. By using Lemma 4.2.1 in (4.1), we note that

$$\mathbb{SO}_\sigma(S_4) = 3(10)^\sigma.$$

Case 2. When $n = 5$ and $b = 1$. By using Lemma 4.2.1 in (4.1), we note that

$$\mathbb{SO}_\sigma(S_5) = 4(17)^\sigma.$$

Case 3. When $n = 13$ and $b = 4$. By using Lemma 4.2.5 in (4.1), we note that

$$\mathbb{SO}_\sigma(T_1) = 9(17)^\sigma + 3(25)^\sigma$$

Case 4. When $2b + 2 \leq n \leq \lfloor \frac{5b+5}{2} \rfloor$ and $b \geq 2$, by using Lemma 4.2.2 in (4.1), we note that

$$\begin{aligned}\mathbb{SO}_\sigma(T_1) = {} & n(3(17)^\sigma - 2(10)^\sigma + (25)^\sigma - (18)^\sigma) + b(-6(17)^\sigma + 5(10)^\sigma - 2(25)^\sigma \\ & + 3(18)^\sigma) - 6(17)^\sigma + 6(10)^\sigma - 2(25)^\sigma + (18)^\sigma.\end{aligned}$$

Case 5. When $\lceil \frac{5b+6}{2} \rceil \leq n \leq \lfloor \frac{8b+7}{3} \rfloor$ and $b \geq 6$, by using Lemma 4.2.3 in (4.1), we note that

$$\begin{aligned}\mathbb{SO}_\sigma(T_1) = {} & n((17)^\sigma + 3(25)^\sigma - 3(18)^\sigma) + b(-(17)^\sigma - 7(25)^\sigma + 8(18)^\sigma) - 8(25)^\sigma \\ & + 7(18)^\sigma.\end{aligned}$$

Case 6. When $\lceil \frac{8b+8}{3} \rceil \leq n \leq 3b + 2$ and $b \geq 2$, by using Lemma 4.2.4 in (4.1), we note that

$$\begin{aligned}\mathbb{SO}_\sigma(T_1) = {} & n((17)^\sigma - 3(25)^\sigma + 3(32)^\sigma) + b(-(17)^\sigma + 9(25)^\sigma - 8(32)^\sigma) + 6(25)^\sigma \\ & - 7(32)^\sigma.\end{aligned}$$

Case 7. When $n \geq 3b + 3$ and $b = 1$, by using Lemma 4.2.7 in (4.1), we note that

$$\mathbb{SO}_\sigma(T_1) = n(8)^\sigma + 3(17)^\sigma + (20)^\sigma + (5)^\sigma - 6(8)^\sigma.$$

Case 8. When $3b+3 \leq n \leq 4b+1$ and $b \geq 2$, by using Lemma 4.2.8 in (4.1), we note that

$$\mathbb{SO}_{\sigma}(T_1) = n(-(32)^{\sigma} + 2(20)^{\sigma}) + b(2(17)^{\sigma} + 4(32)^{\sigma} - 6(20)^{\sigma}) + 2(17)^{\sigma} + (32)^{\sigma} - 4(20)^{\sigma}.$$

Case 9. When $n \geq 4b+2$ and $b \geq 2$, by using Lemma 4.2.9 in (4.1), we note that

$$\mathbb{SO}_{\sigma}(T_1) = n(8)^{\sigma} + b(2(17)^{\sigma} - 4(8)^{\sigma} + 2(20)^{\sigma}) + 2(17)^{\sigma} - (8)^{\sigma} - 2(20)^{\sigma}.$$

This concludes the proof. □

Chemical trees for the maximum general Sombor index correspond to the chemical trees for the maximum general sum-connectivity index given in Theorem 3.2.1 of Chapter 3. Therefore, we omit the construction of trees here.

Summary

Both the general sum-connectivity and general Sombor indices are degree-based topological indices. The general sum-connectivity index is used to study chemical graphs to understand the properties of molecules, such as stability and reactivity. Like the general sum-connectivity index, the general Sombor index is also used in chemical graph theory to study chemical graphs and predict molecular properties.

In the first chapter, we discuss the introduction of graphs, some real-life problems related to graph theory, and the basic terminologies of graphs. The second chapter deals with some degree and distance-based topological indices for a graph which relate a graph to a real number and analysis of general sum-connectivity and general Sombor indices are also discussed. Then in the third chapter, we discussed the maximum values of the general sum-connectivity index in the class $\mathbb{CT}(n, b)$ of chemical trees of order n and b branching vertices. In the last chapter, we discussed the maximum general Sombor index in the class $\mathbb{CT}(n, b)$ of chemical trees.

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