Sombor Index of Some Nanostar Dendrimers and Silicate Structures

By

Nida Ejaz

Supervised by

Dr. Rashid Farooq

National University of Sciences and Technology

School of Natural Sciences (SNS)

Department of Mathematics

Islamabad, Pakistan

2022

FORM TH-4

National University of Sciences & Technology

MS THESIS WORK

We hereby recommend that the dissertation prepared under our supervision by: **Nida Ejaz**, Regn No. **00000321239** Titled: **"Sombor Index of Some Nanostar Dendrimers and Silicate Structures"** accepted in partial fulfillment of the requirements for the award of **MS** degree.

Examination Committee Members

1. Name: DR. MUHAMMAD ISHAQ Signature: _____

2. Name: DR. MUHAMMAD QASIM Signature: _____

Supervisor's Name: PROF. RASHID FAROOQ Signature: _____

_____ 17/06/2022
Head of Department Date

COUNTERSINGED

Date: 17.6.2022 _____
Dean/Principal

Dedicated to
My Loving Parents.

Acknowledgement

First of all, I am grateful to Omnipotent who enabled me to achieve this goal and endowed me immeasurably more than I deserve. Without His support, it was no more than a dream. After that, I am obliged to my supervisor, Dr. Rashid Farooq, who assisted me and guided me at every single stem. Also, I would like to thank my GEC members, Dr. Muhammad Ishaq and Dr. Muhammad Qasim for their kind and undivided attention as well as compassionate consideration. I am thankful to my parents, especially my mother who proved herself as a strong woman and boosted me up throughout the tenure of my study. In addition, I would like to express my gratitude to my spouse Zeshan for his inspiration and support in helping me finish my thesis. lastly, I would like to thank my sisters and nephews Arslan, Usman, Mehran, Farhan, Abdul Moiz, Saad, Abdul Ahad.

Nida Ejaz

Abstract

In 2020, Gutman introduced a degree based topological index of graphs namely the Sombor Index. Let $d_v(G)$ be the degree of the vertex v in graph G. The Sombor Index of G is defined as $SO(G) = \sum_{uv \in \xi(G)} \sqrt{d_u(G)^2 + d_v(G)^2}$. It is a very young field and has gathered the attention of many researchers which has led it to become one of the fundamental concepts of chemical graph theory. In this study, we take into consideration some infinite families of nano star dendrimers such as HFD(ei) dendrimer, Nanostar dendrimers $D_1[n]$, Nanostar dendrimer $D_2[n]$ and Hypercore dendrimerD_n. Compute their Sombor index. Moreover, we find the Sombor index for a few silicate networks like $SLN(n)$ and Chain silicate network CS_n etc.

Contents

Chapter 1

Introduction

In this chapter, we are concerned with the core idea and basic definitions of graph theory. More specifically chemical graph theory is accompanied by various theoretical terms of graph theory. To elaborate on various features of graphs for better understanding, we illustrate the definition along with examples. As graph theory has vast useful applications in chemistry, physics, engineering, architecture, and many other fields so the basic purpose of this chapter is to make it easy for the reader in developing familiarity with the fundamentals of graph theory.

1.1 Graph theory's origins and branches

It is no wonder that the basic idea of graph theory was discovered in the 18th century. Now it is quite properly known as a field of *applied mathematics*.

It came into existence when Leonhard Euler gave the solution to Königsberg's seven bridges problem [25]. The credit of subsequent rediscoveries of it goes to Kirchhoff and Cayley.

Kirchhoff's working on electrical networks led to the development of fundamental concepts and theorems relevant to trees in graphs which we will discuss later. Cayley used trees that arise when he enumeration organic chemical isomers. Another interesting rediscovery to graph theory was set by Hamilton. After that, the famous four-color conjecture came and has been famous ever since [22].

Generally, we can say graph theory is a combinatorics branch but it is the interconnection between applied mathematics and operation research, theory of optimization, organic chemistry, electrical engineering, computer science, civil engineering, and many others. Following are the names of few subbranches of graph theory that attract people of other disciplines towards graph theory.

1. **Chemical graph theory:** Chemical graph theory is an extension of graph theory. It combines chemistry and graph theory. Graph theory works to model mathematically, molecules for gaining insight into the physical properties of given chemical compounds. A few physical properties, like the boiling point, are directly connected to the geometric structure of a given compound. Alexandru Balaban, Haruo Hosoya, Iván Gutman, Ante Graovac, and Milan Randi are some of the pioneers of chemical graph theory [18]. Nenad Trinajsti, Harry Wiener, and a slew of other notables are among them.

2. **Spectral graph theory:** Spectral graph theory is the field of graph theory that studies the properties of a graph along with its *eigenvalues*, *eigenvectors*, and associated *characteristic polynomials*, such as the graph's Laplacian matrix or adjacency matrix. There is some more connection of spectral graph theory with other subjects of mathematics, for example, spectral graph theory has an interesting analogy with differential geometry. Similarly, there is an important

interaction between spectral graph theory and spectral Riemannian geometry.

3. **Algebraic graph theory:** It is an important application of abstract algebra to graph theory. In this particular branch, many important results of graphs can be proved with the aid of using matrices and other algebraic techniques. The use of group theory, together with linear algebra, and the study of graph invariants are the main branches of it.

4. **Topological graph theory:** Graph embedding in surfaces is known as topological graph theory (like $\mathbb{R}^2$, $\mathbb{R}^3$ or on a torus), spatial embeddings of graphs and graphs as itself topological spaces. The term "embedding a graph on a surface" refers to the desire to have a graph on a surface, such as a sphere, with no two edges intersecting. A three-cottage problem is a prime embedding problem that is frequently expressed as a mathematical puzzle. Printing electronic circuits has numerous more uses of topological graph theory. The goal is to create a circuit which is here called “embed” on an electronic circuit board called “surface” without crossing two connections and resulting in a short circuit. It also entails graph immersion research.

5. **Graph coloring:** Graph coloring is not a branch but a special case of graph labeling. It has many applications in daily life so it is treated as specifically a branch of graph theory. Graph coloring is the assignment of colors to every vertex of a graph. But in such a way that no two adjacent vertices are assigned the same color. There are many useful applications of graph coloring which are very interesting to study them for example exam or meeting scheduling, assignment of frequency in radio stations or finding of index registers to store variables temporarily during the execution of the loop, etc.

6. **Optimization problem on graph:** Optimization problems on graphs usually deal with the structure like road network and attempt to minimize cost and maximize flow along with the network. Generally in an optimization problem on graphs, one is asked to give the largest (or smallest) subset of the graph under some given constraints.

1.2 Graphs and its basic terms

A simple graph G is composed of an ordered pair (γ, ξ) of a non-empty set γ and ξ, where the members of γ are referred to as *vertices* (*points*) and the members of ξ are referred to as *edges* (*links*). If edge $e = uv$ then u and v are called *endpoints* or (*end vertices*) of e and e is called *incident edge* to u and v. The cardinality of set γ (respectively ξ) is called *order* (respectively size) of G where the order is denoted by n (or $n(G)$) and size by m (or $m(G)$). For the set of edges, we are referring to write $\xi(G)$ and $\gamma(G)$ for the collection of vertices of G. If two edges of G have the same endpoints, they are called *multiple edges* and if both endpoints are equal for an edge then it is called *loop*. A graph free of loops and multiple edges is called a *simple graph*. A graph having at least a single loop is called a *pseudo graph*. The *line* which connects two vertices say u and v is denoted by $\{u, v\}$ or for more convenience uv (or uv). In a *regular graph* the degree of every vertex is same. If the degree of every vertex in a graph is k then it is called k-regular graph.

The vertices, u and v are called *incident vertices* to e. If two edges share at least one common vertex then they are called *adjacent edges* otherwise called *non-adjacent*. Two vertices in graph G are called *neighbors* or *adjacent vertices* if they are connected by edge. The neighbors of v in G are denoted by $N(v)$ or more clearly $N_G(v)$. This

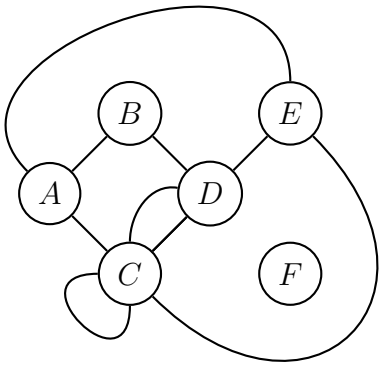


Figure 1.1: graph G_1

set of neighbours $N_G(v)$ is called the *neighborhood* of v. If the set of edges ξ is empty set then graph G is called an *empty graph* or *nullgraph*. The term "*trivial graph*" refers to a graph that has only one vertex and no edges.

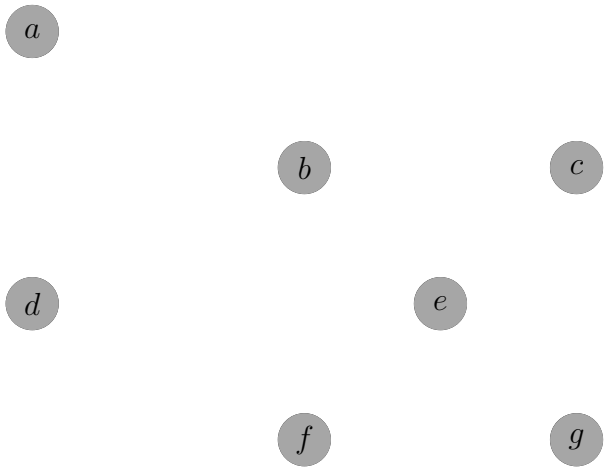


Figure 1.2: Null graph N_7

A *finite graph* is one having both finite order (set of vertices) and size (set of edges), as opposed to an *infinite graph*. G' denotes the *complement* of a simple graph G. It is defined as a simple graph with the same vertex set as G, and an edge satisfying

the property that two vertices are adjacent in G' if and only if they are not adjacent in G. A *undirected graph* has edges but they are not directed edges. In a *directed graph*, each edge has a direction. In a graph G the *degree* of a vertex v is equal to the cardinality of set of neighborhood $N_G(v)$, that is, the number of neighbors of v and it is denoted by d_v. A *regular graph* is a graph where the degree of all its vertices is the same. The *edge degree coordinate* of an edge uv is an ordered pair (d_u, d_v), where u,v are the end vertices of edge uv. In a graph G, $m_{d_u,d_v} = m_{d_u,d_v}(G)$ is the total number of edges joining vertex u of degree d_u with vertex v of degree d_v in G.

Now to elaborate on the above terms defined let us consider few examples. Consider the graph in Figure 1.1. The G_1 graph's set of vertices is $\gamma(G_1)$=$\{A, B, C, D, E, F\}$ so order of graph G_1 is 6. The set of edges of G_1 is $\xi(G_1)$=$\{AB,\ AC,\ AE,\ BD,\ CC,\ CD,\ CD,\ CE,\ DE\}$ so the size of graph G_1 is 9. There are multiple edges between C and D so edge CD is written two times in the edge set. There is a loop on vertex C. The vertex F is called isolated vertex as no edge is incident to it. The neighborhood of $N_G(A)$= $\{\ B,\ C,\ E\ \}$ and $N_G(B)$= $\{A,\ D\}$ and similarly for others. Degrees of A, B, C, D, E, F are $3, 2, 6, 4, 3, 0$ respectively. In counting the degree of a vertex, the loop is counted two times that is why degree of C is 6. The vertices B and E in Figure 1.1 are nonadjacent vertices as there is no edge between them.

Figure 1.2. shows an empty or null graph because it has vertices a, b, c, d, e, f, g but no edge joining them. A bijective function $\emptyset$ between the vertex set of G denoted by $\gamma(G)$ and the vertex set of H denoted by $\gamma(H)$ is called an isomorphism of simple graphs G and H as $\emptyset : \gamma(G) \to \gamma(H)$. In G any two vertices v and u are adjacent if and only if $\emptyset(v)$ and $\emptyset(u)$ are adjacent in H. The bijective mapping of this nature is called "edge-preserving bijection" and the graph G and H are called *isomorphic graph* as shown in Figure 1.3.

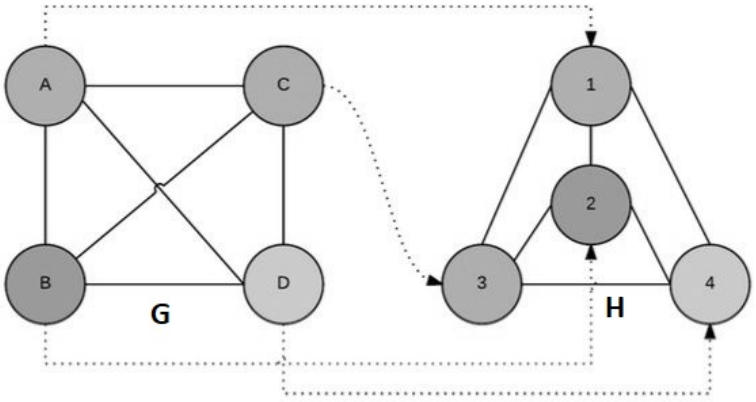


Figure 1.3: Isomorphic graphs G and H

1.2.1 Graph and some related concepts

A *walk* is a finite length alternating sequence of vertices and edges. In a walk, edges and vertices can be repeated. See Figure 1.4. A *trail* is a finite length alternating sequence of vertices and edges. But in a trail, a vertex can be repeated but edges cannot be repeated. See Figure 1.5. If all the edges and vertices are distinct in the walk then it is called a *path*. See Figure 1.6.

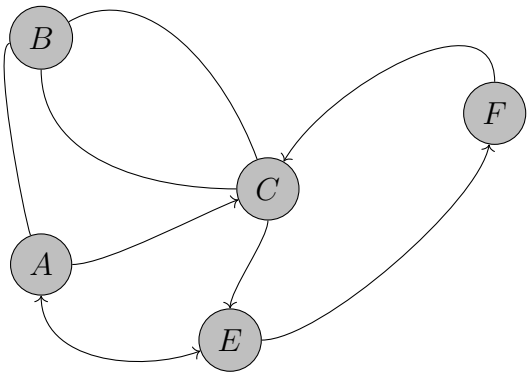


Figure 1.4: walk $AEFCEAC$

In a graph G, a *cycle* is a non-empty trail in which the repeated vertices are only the first and terminal vertex. See Figure 1.7. The length of the smallest cycle in graph

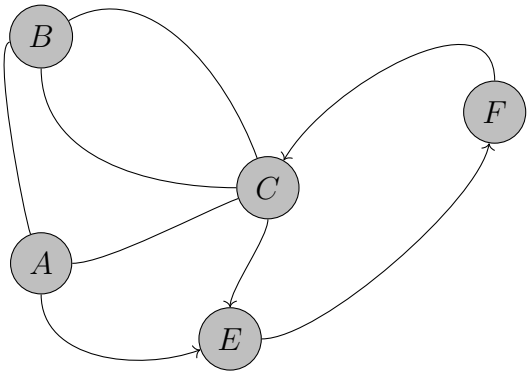


Figure 1.5: trail $AEFCE$

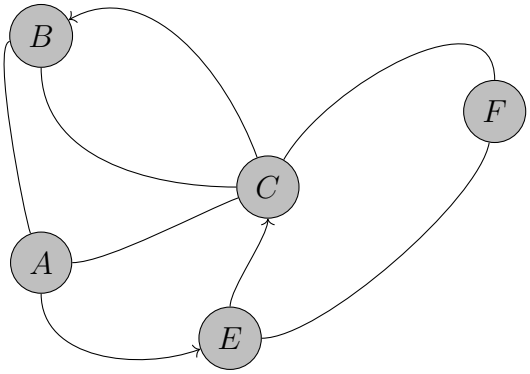


Figure 1.6: path $AECB$

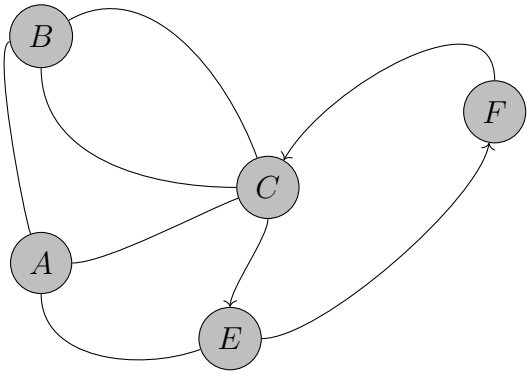


Figure 1.7: cycle $EFCE$

G is called *girth*. It is represented by $\eth(G)$. Also, the length of the largest cycle in G is called the circumference of G. It is denoted by $\zeta(G)$. A *connected graph* is a graph if there exists a path between every pair of vertices of G. Otherwise, graph is called *disconnected*. A *unicyclic graph* is a connected graph that contains only one cycle. Bicyclic graphs are connected graphs that have the same number of edges as vertices plus one.

An *independent set* in graph G is the set of mutually *non-adjacent* vertices in G. The cardinality of the largest independent set is called *independence number*. It is represented by $\nu(G)$.

1.3 Representation of graph in data structure

We can represent a graph in many ways like graphical representation, matrix representation, polynomial representation, numerical representation, etc. A graph is represented in the form of a diagram called graphical representation, however to store a graph as data in a computer's memory, a matrix representation of the graph is commonly used. There are many types of matrices corresponding to graphs. Here we discuss two types of matrix representation. The first is an adjacency matrix while other is an incident matrix.

(a) Representation of a graph by adjacency matrix: If G consists of n vertices then the adjacency matrix of G is an $n \times n$ matrix $A = [a_{ij}]$ and defined by a_{ij}=N if there exists N number of edges between v_i and v_j and $a_{ij} = 0$ otherwise. Note that entries on the main diagonal must be 0 for a simple graph. Here is an example of an adjacency matrix. See Figure 1.8.

(b) Representation of a graph by the incidence matrix: If G consists of n vertices

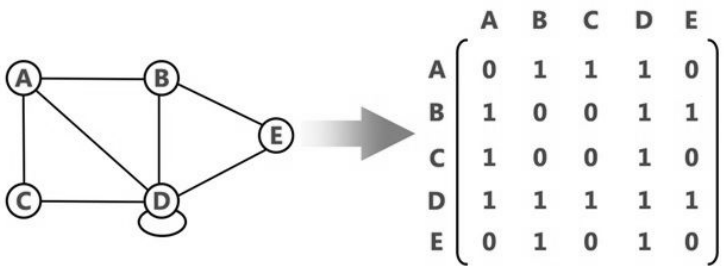


Figure 1.8: Graph G_2 and its adjacency matrix

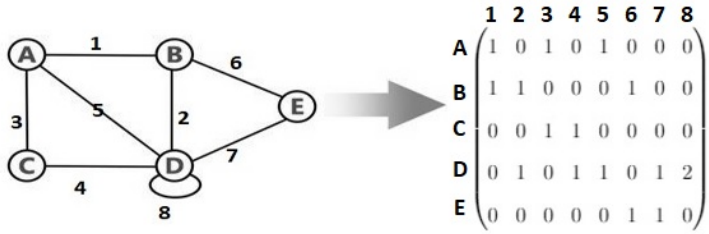


Figure 1.9: Graph G_2 and its incidence matrix

and m edges, then the incidence matrix of G is an $n \times m$ matrix $B = [b_{ij}]$, such that, $b_{ij} = 2$ for self-loop, $b_{ij} = 1$ if the vertex v_i and edge m_j are incident and 0 otherwise. See Figure 1.9.

1.4 Some special types of graphs

If the vertices of a simple graph can be organized in such a way that vertices will be adjacent if and only if they are consecutive in the list, that graph is termed as a *path graph*. The path graph of order n is denoted by P_n. A simple connected graph of order n without having a cycle is called *tree*. See Figure 1.10.

A *star* on n vertices is a tree where $n-1$ vertices are joined to one common n^{th} vertex and denoted by S_n. Figure 1.11 shows an example of a star graph S_9. If every pair of vertices is connected by an edge, such graph is called *complete graph*. A

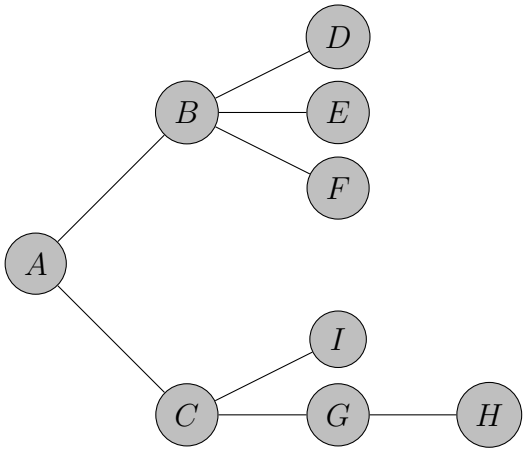


Figure 1.10: Tree on 9 vertices

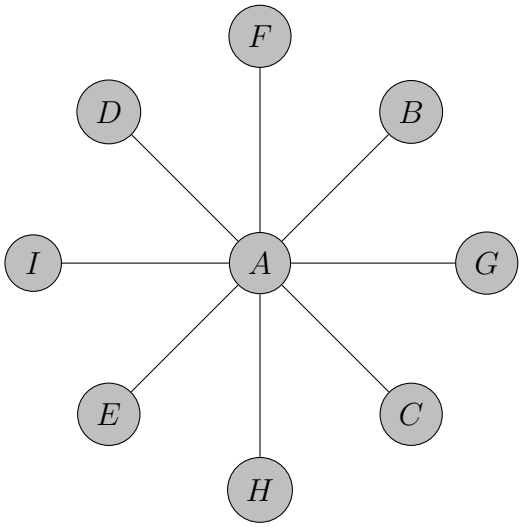


Figure 1.11: Star graph S_9

complete graph is symbolized by K_n if it has order n. The formula to calculate the edges of K_n is defined as $\frac{n(n-1)}{2}$. A simple graph $G = (\gamma, \xi)$ is *bipartite* graph $G(\alpha, \beta)$ if there exists $\alpha \subset \gamma$ and $\beta = \gamma$ - α, such that, every edge has one vertex in α and one in β. See Figure 1.13.

A bipartite graph $G(\alpha, \beta)$ is said to be a *complete bipartite graph* if every vertex in α must be adjacent to every vertex in β. A *semi-regular* or *biregular* is a bipartite

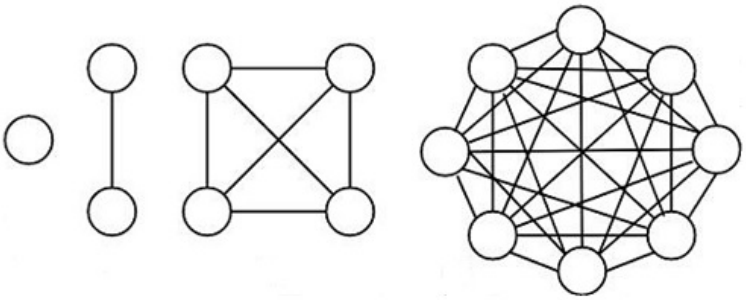


Figure 1.12: complete graph K_1, K_2, K_4, K_8

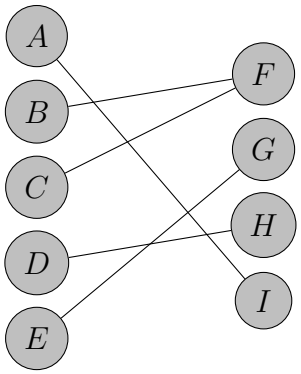


Figure 1.13: Bipartite graph

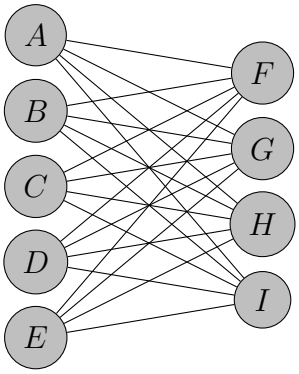


Figure 1.14: Complete bipartite graph

graph $G(\alpha, \beta)$ for which every two vertices on the same side of the given bipartition have the same degree as each other. See Figure 1.14. A regular graph is one in which each vertex has the same number of neighbours, i.e. each vertex has the same degree or valency. A *wheel graph* W_n of order n is a graph obtained by joining a single new

vertex to each vertex of cyclic graph C_{n-1} of order $n-1$. See Figure 1.15. Let G be a k-cyclic graph with k=1, 2. The minimum k-cyclic subgraph $\tilde{G}$ of a k-cyclic graph G is called its base. $\tilde{G}$ is the only k-cyclic subgraph of G that does not contain a pendent vertex, and G can be made from $\tilde{G}$ by adding trees to some or all of G's vertices.

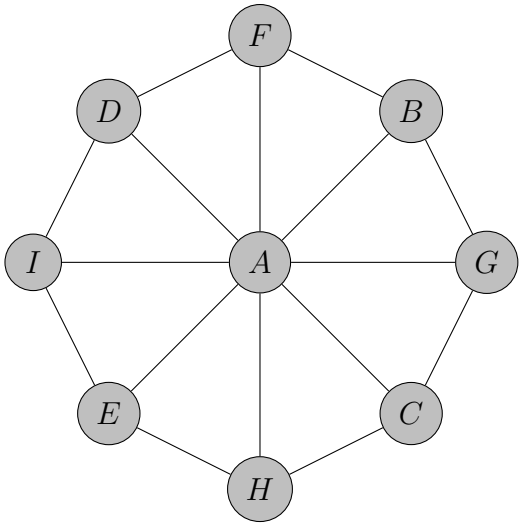


Figure 1.15: Wheel graph

1.5 Theory of chemical graphs

A branch of graph theory called *chemical graph theory* is the application of graph theory in the field where molecular structures matter. This type of study lies under *theoretical chemistry* from the chemistry point of view. We can say chemical graph theory deals with the mathematical modeling of chemical structures (molecules). It has wide applications in $QSPR$ (Quantitative structure–activity relationship) and $QSAR$ (Quantitative structure-property relationship) due to this property. The basic goal of chemical graph theory is to reduce the topological structure of a molecule to a single number by using algebraic invariants which characterize either the energy of the

molecule as a whole or its orbitals, its electronic structures, its structural fragments and, molecular branching among others.

Some of the pioneers of chemical graph theory are Nenad Trinajstić , Ante Graovac, Haruo Hosoya, Iván Gutman, Milan Randić, Alexandru Balaban, Harry Wiener [18].

Molecules and molecular structures are modelled with the help of a graph. Such a graph that is used to characterize a molecule is called a *chemical graph*. *Topological indices* quantify the structure that has been modelled. Topological indices are used to corelate certain pharmacological, toxicological, physicochemical types of properties of chemical compounds. Later, we will explain topological indices in detail. To relate chemistry and graph theory, few equivalence terminologies are used between these two branches like vertices of the graph correspond to atoms in a molecule while edge between vertices corresponds to chemical bonds between atoms of the molecule. Similarly, the degree of vertices corresponds to the valency of atoms. As shown in Table 1.1.

Terms in graph theory	**Terms in chemistry**
Simple connected graph	Molecular graph
Edge	Chemical bond
Vertex	Atom
Degree of a vertex	Valency of an atom

Table 1.1: Equivalence between theoretical terms of graph theory and chemical terms

Frequently studied chemical graphs in chemical graph theory are given as:

- Dendrimers: These are repetitive branch like structures.
- Nano-tubes: Carbon molecules arranged in structure like tube.
- Nano-cones: Carbon molecules arranged in cone like structure.
- Nano-torus: Carbon molecule arranged in doughnut like structure.

- Fullerenes: Carbon molecules arranged in hollow structures, most commonly spheres, tubes, ellipsoids etc.
- Silicate networks: It is a tetrahedral network formed by carbon and oxygen.

1.5.1 Topological indices

Graph-theoretical indices called *topological indices* are numerical invariants. They are linked with the topological characterization of a chemical compound. Topological characterization means these indices relate to different chemical properties of a compound like pharmacological, toxicological, and physicochemical properties. These properties give a quantitative measure of how a specific compound will behave. There is no method to co-relate and compare the results numerically before the invention of topological indices.

A topological index from a mathematical point of view is a function $\varnothing$ from a class of finite graphs F to real numbers $\mathbb{R}$, that is, $\varnothing : F \to \mathbb{R}$ such that if G and H are isomorphic graphs to each other then $\varnothing(G) = \varnothing(H)$. The use of calculating topological indices is not only to verify the existing properties of a certain chemical compound but these indices can also be used to design compounds with particularly required properties.

There exist more than 150 topological indices. Topological indices are classified into different types, based upon parameters used in them.

- Degree based topological indices.
- Eccentricity based topological indices.
- Distance based topological indices.

- Spectrum based topological indices.

But in our study we only focus on degree based topological indices.

Degree based topological indices

Degree based topological indices are defined by using the degree of vertices in a graph. Degree based topological index is defined as:

$$TI(G) = \sum_{e_{ij} \in \xi(G)} f(degr(v_i), degr(v_j)), \tag{1.1}$$

where f is a symmetric function, that is,

$$f(degr(v_i), degr(v_j)) = f(degr(v_j), degr(v_i)).$$

Some of the degree based topological indices are listed. See Table 1.2.

$f(d_{v_i}, d_{v_j})$	Name of index
$d_{v_i} + d_{v_j}$	First Zagreb index
$d_{v_i} d_{v_j}$	Second Zagreb index
$\lvert d_{v_i} - d_{v_j} \rvert$	Albertson index
$(d_{v_i} + d_{v_j})^2$	First hyper-Zagreb index
$(d_{v_i} d_{v_j})^2$	Second hyper-Zagreb index
${d_{v_i}}^2 + {d_{v_j}}^2$	Forgotten index
$(\frac{d_{v_i}}{d_{v_j}} + \frac{d_{v_j}}{d_{v_i}})/2$	Extended index
$\sqrt{d_{v_i} d_{v_j}}$	Reciprocal Randić index
$1/\sqrt{d_{v_i} d_{v_j}}$	Randić index
$\sqrt{d_{v_i} + d_{v_j}}$	Reciprocal sum-connectivity Randić index
$1/\sqrt{d_{v_i} + d_{v_j}}$	Sum-connectivity Randić index
$1/d_{v_i} + d_{v_j}$	Harmonic index
${d_{v_i}}^{-2} + {d_{v_j}}^{-2}$	Inverse degree index
$\sqrt{(d_{v_i} + d_{v_j}) d_{v_i} d_{v_j}}$	Product connectivity Gourava index
$1/\sqrt{d_{v_i} + d_{v_j} + d_{v_i} d_{v_j}}$	Sum connectivity Gourava index
$[d_{v_i} + d_{v_j} + d_{v_i} d_{v_j}]^2$	First hyper- Gourava index
$[\sqrt{(d_{v_i} + d_{v_j}) d_{v_i} d_{v_j}}]^2$	Second hyper- Gourava index
$d_{v_i} + d_{v_j} + d_{v_i} d_{v_j}$	First Gourava index
$(d_{v_i} + d_{v_j}) d_{v_i} d_{v_j}$	Second Gourava index
$\sqrt{(d_{v_i} + d_{v_j} - 2)/d_{v_i} d_{v_j}}$	Atom-bond connectivity index
$(d_{v_i} + d_{v_j})/(2\sqrt{d_{v_i} d_{v_j}})$	Arithmetic-geometric index
$2\sqrt{d_{v_i} d_{v_j}}/(d_{v_i} + d_{v_j})$	Geometric-Arithmetic index
$(d_{v_i} - d_{v_j})^2$	Sigma index
$d_{v_i} d_{v_j}/(d_{v_i} + d_{v_j} - 2)$	Augmented Zagreb index
$1/\sqrt{d_{v_i} + d_{v_j}}$	Sum connectivity index
$\sqrt{d_{v_i} + d_{v_j}}$	Reciprocal sum connectivity index
$\sqrt{{d_{v_i}}^2 + {d_{v_j}}^2}$	Sombor index

Table 1.2: Degree based topological indices

Chapter 2

Review of Sombor index

2.1 Introduction

Consider a simple graph G with vertex set $\gamma(G)$ and edge set $\xi(G)$. If G has an edge uv with end points u, v then Sombor index of G is defined as [11]:

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

where d_u, d_v are the degrees of vertices u and v, respectively. The summation is over all edges in G. The term $\sqrt{{d_u}^2 + d_v^2}$ is interpreted as degree radius of edge uv in G, that is, distance of ordered pair (d_u, d_v) from the origin $(0, 0)$, where $d_u \leq d_v$.

The Sombor index of a graph is a unique vertex degree-based structure descriptor put forward by Gutman [11]. Redžepoviće [19] showed that the Sombor index is used efficiently in modeling characteristic thermodynamic properties of compounds. It has the satisfactory potential of prediction in modeling the enthalpy of vaporization and entropy of alkanes. Wang et al. [24] and Das et al. [6] calculated the relationship be-

tween the Sombor index and some other degree-based topological indices like forgotten index, the first Zagreb index, second Zagreb index, etc. The relationship between the Sombor index and Albertson index is used to quantifying graph irregularity [1, 21], which we will discuss later.

Definition 2.1.1 ([11]). *The ordered pair (d_u, d_v), where $d_u \leq d_v$ is degree-coordinate of edge $uv \in \xi(G)$. In the two dimensional coordinate system it is considered as a point called degree-point or d-point of an edge uv.*

Definition 2.1.2 ([11]). *The point with coordinate (d_v, d_u) is called dual-degree or dd-point of the edge uv.*

Definition 2.1.3 ([11]). *The distance between degree-point (d_u, d_v) and the origin $(0, 0)$ is the d-radius or degree-radius of edge uv and denoted by $r(d_u, d_v)$, that is,*

$$r(d_u, d_v) = \sqrt{(d_u - 0)^2 + (d_v - 0)^2}$$

It is clear from above equation that degree-point and the corresponding dual degree-point have equal degree-radii. Also in [11] Gutman established another interesting relationship. Consider d-point of an edge uv of the graph. The distance between degree-point (d_u, d_v) and corresponding dual degree-point (d_v, d_u) is given by

$$\sqrt{(d_u - d_v)^2 + (d_v - d_u)^2} = \sqrt{2}|d_u - d_v|.$$

By applying summation on both sides, we obtain

$$\sum_{uv \in \xi(G)} \sqrt{(d_u - d_v)^2 + (d_v - d_u)^2} = \sqrt{2} \sum_{uv \in \xi(G)} |d_u - d_v|.$$

The above equation shows that sum of the distances between d-point and dd-point of the underlining graph is just $\sqrt{2}$ times the Albertson index [21] defined as

$$AI(G) = \sum_{uv \in \xi(G)} |d_u - d_v|.$$

Thus, now the earlier studied Albertson index is used to quantify graph irregularity [1, 21], which can be interpreted as the sum of the distances between degree-points and dual degree-points of a specific graph.

2.2 Relationship of Sombor index with some other topological indices

2.2.1 The first Zagreb index and the Sombor index

Theorem 2.2.1 ([6]). *Let G be a graph of minimum degree δ and size m. Then*

$$SO(G) \leq (\sqrt{2} - 2)\delta m + Z_1(G),$$

where $Z_1(G)$ is the first Zagreb index of G. In addition, the equality holds if and only if graph G is a regular.

2.2.2 Sombor index and second Zagreb index

Theorem 2.2.2 ([6]). *Let G be a graph of order n. Suppose G has minimum degree δ and maximum degree Δ. Then we obtain*

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

where $Z_2(G)$ is the second Zagreb index of G. Moreover, equality holds if and only if graph G is regular.

2.2.3 Sombor index and Randić index

For graph G, Randić index [15, 17] is defined as

$$R(G) = \sum_{uv \in \xi(G)} 1/\sqrt{d_u d_v}.$$

For a graph G, reciprocal randic index [9, 10] is defined as

$$RR(G) = \sum_{uv \in \xi(G)} \sqrt{d_u d_v}$$

Also, there exists an interesting relationship between Randić index and reciprocal Randić index [9, 10]. For any graph G of size m, it holds that

$$RR(G) \times R(G) \geq m^2,$$

where equality holds if and only if graph G is regular.

Using the definition of reciprocal Randić index and the above relation between $R(G)$

and $RR(G)$, we have following result.

Theorem 2.2.3 ([20]). *For graph G of size m, it holds that*

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

Equality holds if and only if graph G is regular.

2.3 Sombor index of some basic graphs

The Sombor index of a complete graph K_n of order n and its complement K'_n is given [11]:

$$SO(K_n) = \frac{n(n-1)^2}{\sqrt{2}}$$

and

$$SO(K'_n) = 0.$$

The Sombor index of a path P_n of order n is given [11]:

For $n = 2$:

$$SO(P_2) = \sqrt{2}.$$

For $n \geq 3$:

$$SO(P_n) = 2(n-3)\sqrt{2} + 2\sqrt{5}.$$

The Sombor index of star graph S_n of order n is given as [11]:

$$SO(S_n) = (n-1)\sqrt{n^2 - 2n + 2}.$$

The Sombor index of cycle graph C_n is given as [11]:

$$SO(C_n) = (2\sqrt{2})n.$$

Theorem 2.3.1 ([6]). *Let G be a bipartite graph of order n. Then*

$$SO(G) \leq \begin{cases} n^3/\sqrt{32} & \text{if } n \text{ is even} \\ (n^2-1)\sqrt{n^2+1}/\sqrt{32} & \text{if } n \text{ is odd} \end{cases}$$

with equality holds if and only if G is isomorphic to $K_{\lceil \frac{x}{2} \rceil, \lfloor \frac{x}{2} \rfloor}$ (which is complete bipartite graph with two partite sets having coordinality $\lfloor \frac{x}{2} \rfloor$ and $\lceil \frac{x}{2} \rceil$, respectively)

2.4 Some special properties of Sombor index

Theorem 2.4.1 ([11]). *For a class of chemical graphs G if the degree of vertices is maximum 4, then two d-points have equal degree-radii if and only if both have the same d-coordinates.*

Lemma 2.4.1 ([6]). *For any graph G having an edge uv, we have*

$$SO(G - uv) < SO(G).$$

Also, an edge uv where vertices u, v are non-adjacent in G, it holds that

$$SO(G + uv) > SO(G).$$

Theorem 2.4.2 ([6]). *Let G be a graph of order n. Then*

$$SO(G) + SO(G') \leq \frac{(n-1)n}{\sqrt{2}}.$$

Equality holds if and only if G is isomorphic to K_n(complete graph of order n) or K'_n.

Reduced Sombor index

The degree-point of an isolated edge in a graph G is given as $(1, 1)$. The distance between any degree-point of any edge of the graph G and degree-point of isolated edge is called reduced Sombor index [11] written as

$$SO_{reduced}(G) = \sum_{uv \in \xi(G)} \sqrt{(d_u - 1)^2 + (d_v - 1)^2}.$$

Average Sombor index

For a graph G of size m and order n, the average vertex degree is $\frac{2m}{n}$. Such degree point has coordinate $(\frac{2m}{n}, \frac{2m}{n})$. The distance between average degree-point and the degree-points of the graph is called average Sombor index and is given as:

$$SO_{average}(G) = \sum_{uv \in \xi(G)} \sqrt{(d_u - \frac{2m}{n})^2 + (d_v - \frac{2m}{n})^2}.$$

It is clear that the above equation is equal to zero if G is a regular graph and it will be positive if graph G is not regular. Thus we can consider $SO_{average}(G)$ to check graph irregularity [1, 21].

2.5 Some results on Sombor index

Finding the extremal values of topological indices is of great interest in mathematical chemistry. Due to which the extremal values of the Sombor index of graphs have quickly received much attention. In the beginning, Gutman [11] calculated extremal values of the Sombor index among the class of trees and other connected graphs. Then Cruz et al. [4] obtained extremals of Sombor index over chemical trees, chemical graphs, and hexagonal systems. Deng et al. [7] studied the upper bounds of the Sombor index over molecular trees with a fixed order. Liu [14] determined minimal of first fourteen chemical trees, the first four unicyclic graphs, the first three chemical bicyclic graphs, and the first seven chemical tricyclic graphs. Lin et al. [16] calculated upper and lower bounds on energy, Estrada index, and the spectral radius of Sombor matrix of graphs. Also characterized respective extremal graphs. Similarly, Ting et al. [26] calculated the Sombor index of unicyclic graphs and trees with a fixed maximum degree.

Theorem 2.5.1 ([11]). *For any graph G of order n,*

$$SO(K_n') \leq SO(G) \leq SO(K_n),$$

where K_n be a complete graph over n vertices, and K_n' be its complement. Equality holds if and only if $G \cong K_n$ or $G \cong K_n'$.

Theorem 2.5.2 ([11]). *For any connected graph G of order n,*

$$SO(K_n) \geq SO(G) \geq SO(P_n),$$

where K_n be the complete graph of order n and P_n be the path of order n. Equality holds if and only if G is isomorphic to K_n or P_n.

Theorem 2.5.3 ([11]). *Let S_n be the star graph of order n. Then for any tree T_n of order n, we have*

$$SO(S_n) \geq SO(T_n) \geq SO(P_n).$$

Equality holds if and only if tree T_n is isomorphic to S_n or P_n.

Theorem 2.5.4 ([6]). *Let G be any graph of order n. If G has minimum degree δ and maximum degree Δ, then*

$$n\delta^2/\sqrt{2} \leq SO(G) \leq n\Delta^2/\sqrt{2}.$$

Equality holds if and only if G is a regular graph.

Upper bounds of Sombor index for different graphs

Theorem 2.5.5 ([6]). *Let G be a connected graph of order n and independence number ν. Then*

$$SO(G) \leq \sqrt{2}\binom{n-\nu}{2}(n-1) + \nu(n-\nu) \times \sqrt{(n-1)^2 + (n-\nu)^2}.$$

Equality holds if and only if G is isomorphic to complete split graph $CS(n, \nu)$.

Theorem 2.5.6 ([5]). *For any unicyclic graph G of order $n \geq 4$, we have*

$$SO(G) \leq SO(U^*(n, n-3, 0, 0)),$$

where $U^*(n, n-3, 0, 0)$ is shown in Figure 2.1.

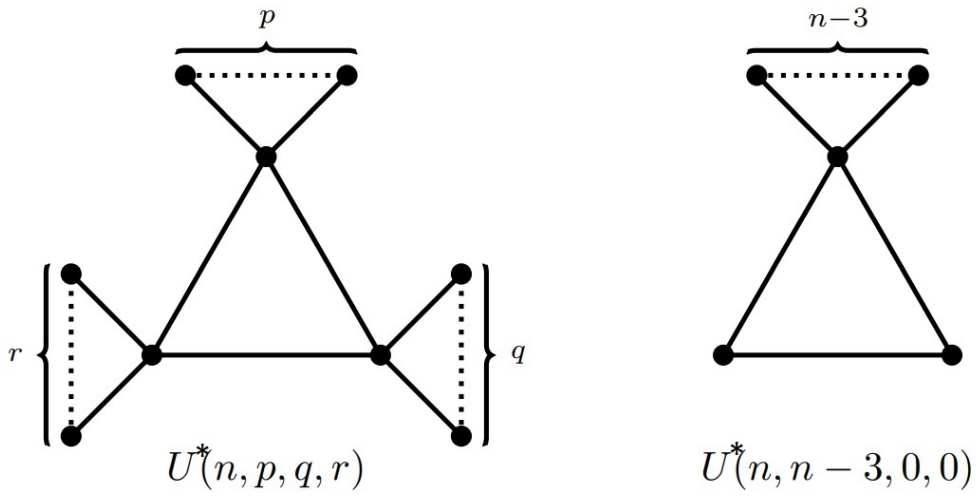


Figure 2.1: Graph $U^*(n,p,q,r)$

Theorem 2.5.7 ([5]). *For any bicyclic graph G of order $n \geq 6$, we have*

$$SO(G) \leq SO(B^*_{2,0}(n, n-4, 0, 0, 0)),$$

where $B^*_{2,0}(n, n-4, 0, 0, 0)$ is shown in Figure 2.2.

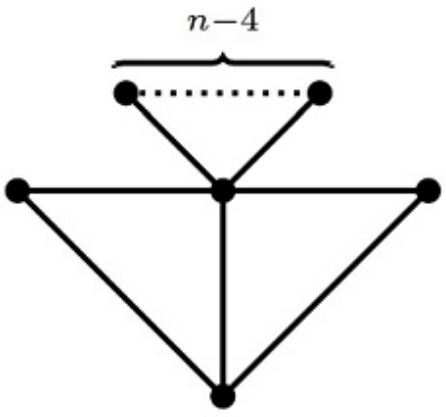
Lower bounds of Sombor index for different graphs

Theorem 2.5.8 ([20]). *For a graph G of order $|\gamma(G)| = n$ and size $|\xi(G)| = m$, we have*

$$2\sqrt{2}m^2/n \leq SO(G).$$

Theorem 2.5.9 ([5]). *If G belongs to the class of unicyclic graphs of order n, then*

$$SO(C_n) \leq SO(G),$$



$B^*_{2,0}(n, n-4, 0, 0, 0)$

Figure 2.2: Graph $B^*_{2,0}(n, n-4, 0, 0, 0)$

where C_n is a cyclic graph.

If G belongs to the class of bicyclic graphs, then G contains two cycles C and C'. The set of bicyclic graphs of order n has three types of bases B_0, B_1 and B_2. The bases B_0, B_1 and B_2 are depicted in Figure 2.3. $B_0(n)$ denotes the set of graphs in B_0

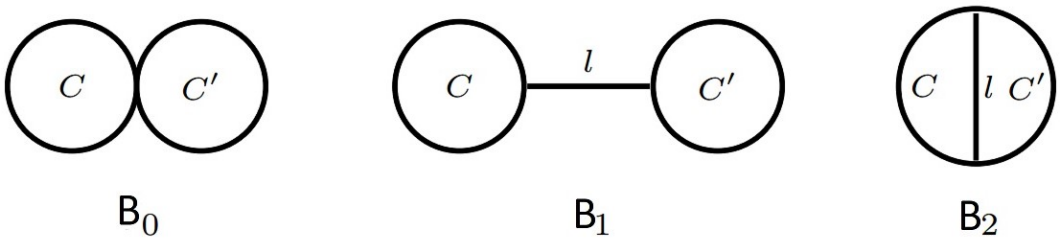


Figure 2.3: Basis of bicyclic graphs

of order n. $B_1(n, l)$ denotes the set of graphs in B_1, where $l \geq 1$ is the length of the path connecting cycles C and C'. $B_2(n, l)$ denotes the set of graphs in B_2 of order n, where $l \geq 1$ is the length of the common path formed by C and C'. The values of the

Sombor index of the graphs in these subclasses are given as:

$$SO(B_0(n)) = 8\sqrt{5} - 6\sqrt{2} + 2\sqrt{2}$$

$$SO(B_1(n,1) \cup B_2(n,1)) = 4\sqrt{13} - 5\sqrt{2} + 2\sqrt{2}$$

$$SO(B_1(n,l>1) \cup B_2(n,l>1)) = 6\sqrt{13} - 10\sqrt{2} + 2\sqrt{2}$$

Theorem 2.5.10 ([5]). *If G belongs to the class of bicyclic graphs of order n, then*

$$SO(\overline{G}) \leq SO(G),$$

where $\overline{G}$ is any graph in $B_1(n,1) \cup B_2(n,1)$.

The maximum value of Sombor index over the set of base bicyclic graphs of order n is attained in $B_0(n)$, while the minimum is attained in $B_1(n,1) \cup B_2(n,1)$.

Sombor index of unicyclic graphs and trees with fixed maximum degree

The graphs $T_{n,\Delta}$, $U_{n,\Delta}$, T_Δ,U_Δ are shown in the Figure 2.4.

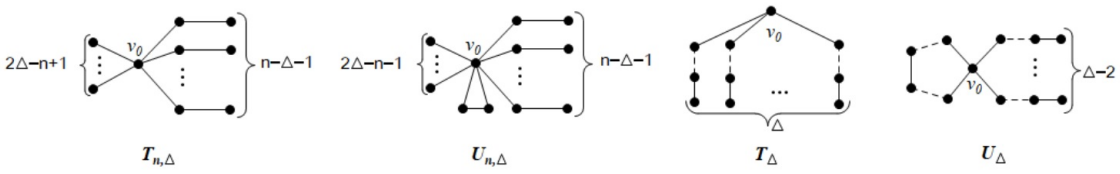


Figure 2.4: The graphs $T_{n,\Delta}$, $U_{n,\Delta}$, T_Δ, U_Δ

Theorem 2.5.11 ([26]). *Let $n \geq 7$ and T belongs to set of trees with n vertices and maximum degree Δ, where $n-2 \geq \Delta \geq 3$.*

(I) With $3 \leq \Delta \leq \left\lfloor \frac{n-1}{2} \right\rfloor$*, we have*

$$\sqrt{5}\Delta + \sqrt{8}(n - 2\Delta - 1) + \Delta\sqrt{\Delta^2 + 4} \leq SO(T).$$

Equality holds if and only if T *is isomorphic to* T_Δ*.*

(II) With $\left\lfloor \frac{n-1}{2} \right\rfloor \leq \Delta \leq n - 2$*, we have*

$$\sqrt{5}(n - \Delta - 1) + (2\Delta - n + 1)\sqrt{1 + \Delta^2} + (n - \Delta - 1)\sqrt{4 + \Delta^2} \leq SO(T).$$

Equality holds if and only if T *is isomorphic to* $T_{n,\Delta}$*.*

Theorem 2.5.12 ([26])**.** *Let* $n \geq 5$ *and* U *belongs to set of unicyclic graphs with* n *vertices and maximum degree* Δ*, where* $3 \leq \Delta \leq n - 2$*.*

(I) With $3 \leq \Delta \leq \left\lfloor \frac{n-1}{2} \right\rfloor$*, we have*

$$\sqrt{5}(\Delta - 2) + \sqrt{8}(n - 2\Delta + 4) + \Delta\sqrt{\Delta^2 + 4} \leq SO(U).$$

Equality holds if and only if U *is isomorphic to* U_Δ*.*

(II) With $\left\lfloor \frac{n-1}{2} \right\rfloor \leq \Delta \leq n - 2$*, we have*

$$\sqrt{8} + \sqrt{5}(n - \Delta - 1) + (2\Delta - n - 1)\sqrt{1 + \Delta^2} + (n - \Delta + 1)\sqrt{4 + \Delta^2} \leq SO(U).$$

Equality holds if and only if U *is isomorphic to* $U_{n,\Delta}$*.*

2.6 Extremal values of chemical graphs w.r.t. Sombor index

Theorem 2.6.1 ([4]). *Let G be a chemical graph of order $|\gamma(G)| = n$. Then*

$$SO(G) = n \times 8\sqrt{2}.$$

Equality holds if and only if G is four-regular graph.

Chemical trees

The chemical tree is a tree whose vertex degree cannot exceed 4.

Theorem 2.6.2 ([4]). *Let G be a chemical tree of order $|\gamma(G)| = n$. Then*

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

Equality holds in the left side if and only if G is isomorphic to P_n. The equality holds in the right if and only if G is isomorphic to 4-regular graph.

Theorem 2.6.3 ([4]). *Let T_n be a chemical tree with order $n \geq 3$. Then*

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

Equality holds if and only if T_n is without vertex of degree 2 and 3.

Three special types of chemical graphs

If G is a chemical graph with no isolated vertex then n_x=$n_x(G)$ denotes the total number of vertices of G having vertex degree x. In the chemical graph G, $m_{x,y}$=$m_{x,y}(G)$ is the total number of edges joining a vertex of degree x with vertex of degree y in G. Now we have three special types of chemical connected graph based on which we will state next theorems.

Theorem 2.6.4 ([4]). *Let n be a positive integer. Then, among all chemical trees of order n, the maximal value of Somber index is attained in:*

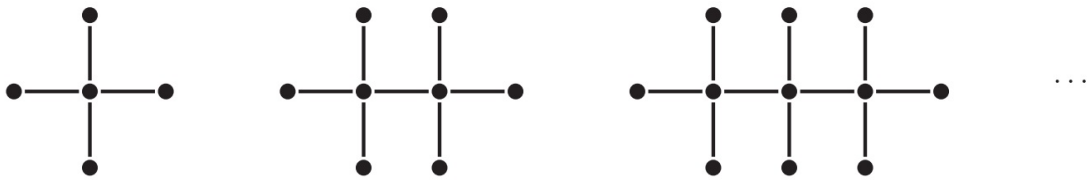


Figure 2.5: C_{00} type of trees

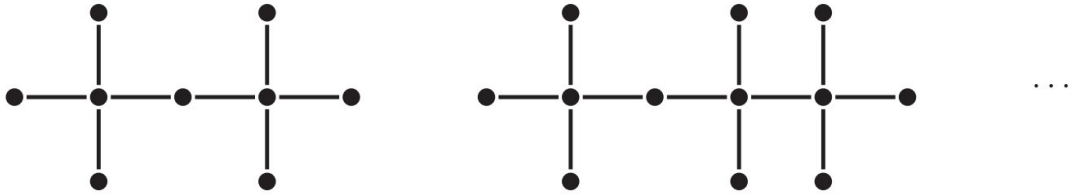


Figure 2.6: C_{10} type of trees

1. $T \in C_{00}(n)$ *if* $n \equiv 2$ *(mod 3) for* $n \geq 5$

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

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

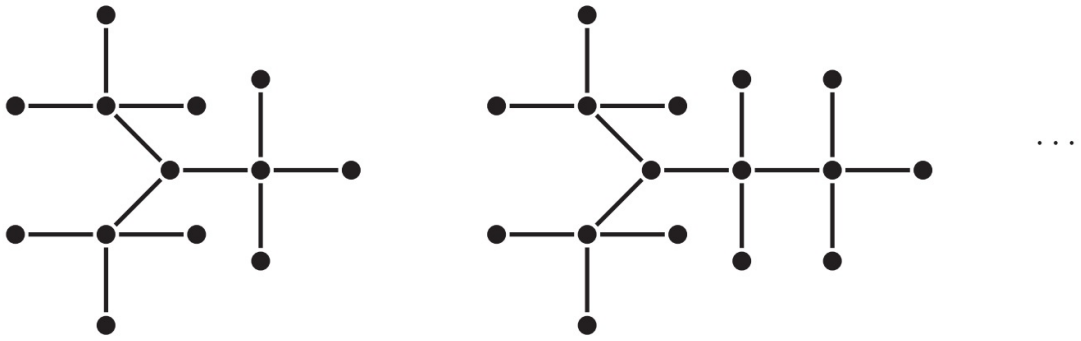


Figure 2.7: C_{01} type of trees

Theorem 2.6.5 ([26]). *Let T be a chemical tree of order $n \geq 7$. If maximum degree of T is $\Delta = 3$, then*

$$3\sqrt{13} + 2\sqrt{2}n + 3\sqrt{5} - 14\sqrt{2} \leq SO(T).$$

Equality holds if and only if $T \cong T_3$. If $\Delta = 4$, then

$$2\sqrt{2}n - 6\sqrt{2} \leq SO(T).$$

Equality holds if and only if $T \cong T_4$.

Theorem 2.6.6 ([26]). *Let T be a chemical unicyclic graph of order $n \geq 5$. If $\Delta = 3$, then*

$$3\sqrt{13} + 2\sqrt{2}n + \sqrt{5} - 4\sqrt{2} \leq SO(T).$$

Equality holds if and only if $T \cong U_3$. If $\Delta = 4$, then

$$2\sqrt{2}n + 10\sqrt{5}_8\sqrt{2} \leq SO(T).$$

Equality holds if and only if $T \cong U_4$.

Integer valued Sombor index of graphs

Proposition 2.6.7 ([20]). *Let* G *a connected chemical graph with no isolated vertex. Then Sombor index of* G *is an integer if and only if* G *is a biregular bipartite graph with* $\Delta = 4$ *and* $\delta = 3$. *Also,*

$$SO(G) = 5|\xi(G)|.$$

Theorem 2.6.8 ([20]). *Let* G *be a connected graph and let Sombor index of* G *be an integer. Then* G *must be multi-partite graph with* δ *is at-least 3.*

2.7 Future work directions on Sombor index

In the last section we have indicate some possible directions for further work in Somber index. Also some concluding remarks have been offered.

p-Sombor index

Beyond Euclidean norm that was used by Ivan [11] in defining Sombor index, the most obvious case is *p-variant* Sombor index defined as

$$SO_p(G) = \sum_{uv \in \xi(G)} ({d_u}^p + d_v^p)^{1/p},$$

where $p \neq 0$. So we can find extremals and other results of sombor index for p-Sombor index. Few of them are given below:

Proposition 2.7.1 ([4]). *If G is a simple graph with $0 < p < q$, then*

$$SO_q(G) < SO_p(G).$$

Proposition 2.7.2 ([4]). *For a simple graph G with $p > 2$ be an integer then p-Sombor index of G is not an integer.*

Proposition 2.7.3 ([4]). *For any graph G*

$$SO_{\frac{1}{2}}(G) = Z_1(G) + 2RR(G),$$

where $Z_1(G)$ is first zagreb index and $RR(G)$ is reciprocal randic index.

Proposition 2.7.4 ([4]). *For a graph G with no isolated vertex then*

$$\lim_{p \to 0} SO_p(G) = \infty.$$

It is interesting that we also have results for $p < 0$ such that for $p = -1$ we have

$$SO_{-1}(G) = \text{Inverse sum indeg index}.$$

See [23] for more about inverse sum indeg index.

Chapter 3

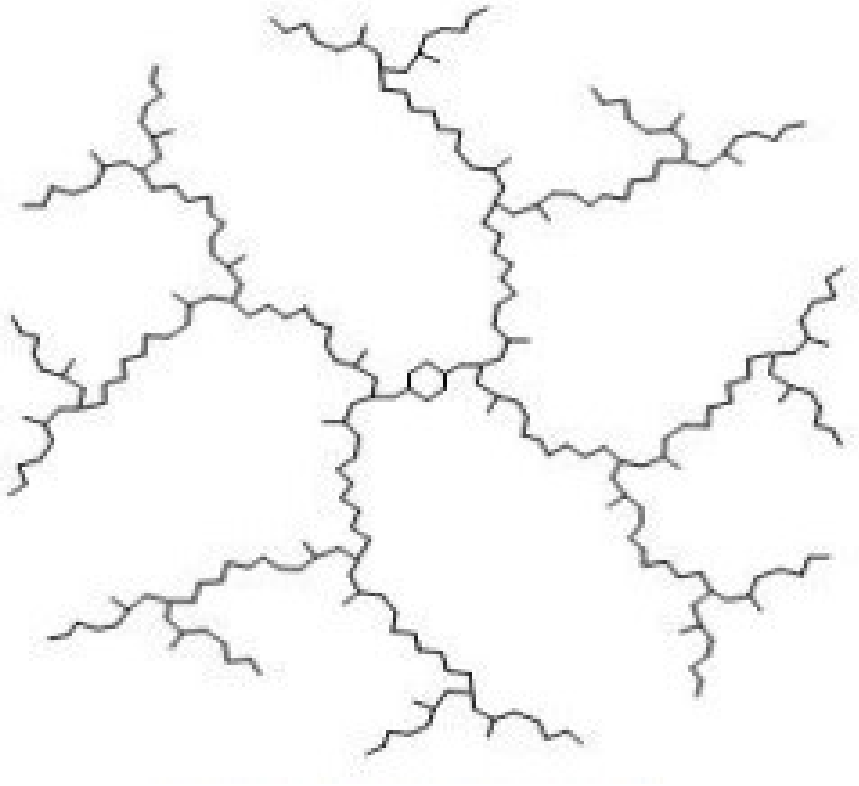
Sombor index of some dendrimers

3.1 HFD(ei) dendrimer

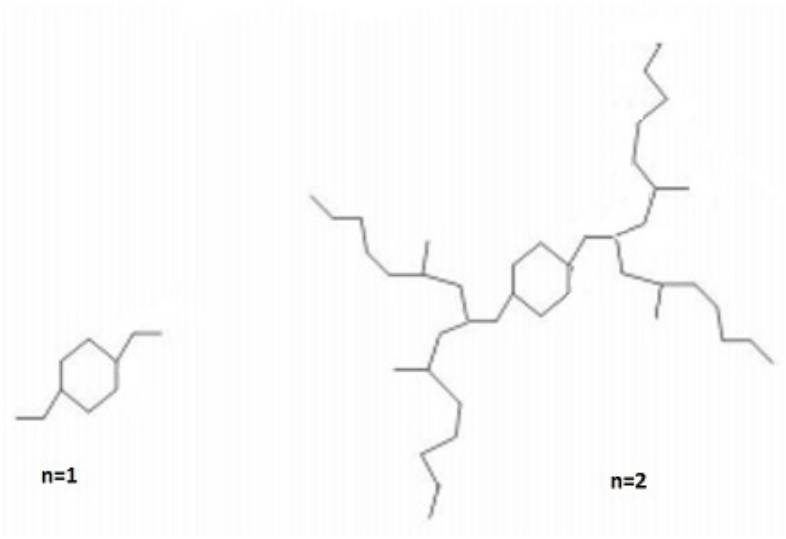
In this section, we will calculate the Sombor index of a dendrimer named as HFD(ei)-G3-e(allyl)16-i-(hydroxyl)28, which is denoted by $D[n]$ as shown in Figure 3.1 with different stages of its growth.

Theorem 3.1.1. *For $HFD(ei) - G3 - e(allyl)16 - i - (hydroxyl)28$ dendrimer, the Sombor index is given as*

$$SO(D[n]) = \begin{cases} 2[\sqrt{5} + \sqrt{8} + 3\sqrt{13}] & for \;\; n = 1 \\ 2^{t+1}[\sqrt{5} + 10\sqrt{8} + 2\sqrt{10} + 7\sqrt{13}] - [4\sqrt{10} \\ +26\sqrt{8} + 8\sqrt{13}] & for \;\; n = 2t, t \geq 1 \\ 2^{t+1}[\sqrt{5} + 14\sqrt{8} + 2\sqrt{10} + 7\sqrt{13}] - [4\sqrt{10} \\ +26\sqrt{8} + 8\sqrt{13}] & for \;\; n = 2t+1, t \geq 1 \end{cases}$$



(a) D[n] with $n = 6$



(b) $D[n]$ with $n = 1, 2$

Figure 3.1: Represent different stages of growth of HFD

Proof. We know that formula of Sombor index is given as:

$$SO(D[n]) = \sum_{uv \in \xi(D[n])} \sqrt{{d_u}^2 + d_v^2}.$$

Let

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

Then

$$SO(D[n]) = \sum_{(u,v) \in B} \sqrt{{d_u}^2 + d_v^2}\ m_{u,v}, \tag{3.1}$$

where $m_{u,v}$ is the number of edges with end points u and v.

HFD are the macro-molecules, due to molecular structure degree of vertices cannot exceed 4 so we have,

$$\begin{aligned} SO(D[n]) =& \sqrt{1^2+1^2}m_{1,1} + \sqrt{1^2+2^2}m_{1,2} + \sqrt{1^2+3^2}m_{1,3} + \sqrt{1^2+4^2}m_{1,4} \\ &+ \sqrt{2^2+2^2}m_{2,2} + \sqrt{2^2+3^2}m_{2,3} + \sqrt{2^2+4^2}m_{2,4} + \sqrt{3^2+3^2}m_{3,3} \\ &+ \sqrt{3^2+4^2}m_{3,4} + \sqrt{4^2+4^2}m_{4,4}. \end{aligned}$$

We can see from the Figure 3.1 that all the edges of $D[n]$ has degree coordinats of the type $(1,2), (1,3), (2,2), (2,3)$. So the number of all the other type of edges will be equal to zero.

$$\begin{aligned} SO(D[n]) =& \sqrt{1^2+1^2}(0) + \sqrt{1^2+2^2}m_{1,2} + \sqrt{1^2+3^2}m_{1,3} + \sqrt{1^2+4^2}(0) \\ &+ \sqrt{2^2+2^2}m_{2,2} + \sqrt{2^2+3^2}m_{2,3} + \sqrt{2^2+4^2}(0) + \sqrt{3^2+3^2}(0) \\ &+ \sqrt{3^2+4^2}(0) + \sqrt{4^2+4^2}(0) \end{aligned} \tag{3.2}$$

The number of edges of $D[n]$ is equal to $16(2^{t+1}) + 8(2^t) - 38$ if $n = 2t, t \geq 1$ and $24(2^{t+1}) - 38$ if $n = 2t + 1, t \geq 0$. First we calculate Sombor index for first growth of $HFD(ei) - G3 - e(allyl)16 - i - (hydroxyl)28$ dendrimer $D[n]$. It is clear from Figure 3.1 that edge partition for $n = 1$ is

(d_u, d_v) where $uv \in D[1]$	$(1,2)$	$(1,3)$	$(2,2)$	$(2,3)$
$Numberofedges$	2	0	2	6

Table 3.1: Edge partition of $D[1]$ based on the degrees of end vertices of every single edge with $n = 1$

By putting the values in equation 3.2, we have

$$\begin{aligned} SO(D[1]) &= \sqrt{1^2+2^2} \times 2 + \sqrt{1^2+3^2} \times 0 + \sqrt{2^2+2^2} \times 2 + \sqrt{2^2+3^2} \times 6 \\ &= \sqrt{5} \times 2 + \sqrt{8} \times 2 + \sqrt{13} \times 6 \\ &= 2\sqrt{5} + 2\sqrt{8} + 6\sqrt{13} \\ &= 2[\sqrt{5} + \sqrt{8} + 3\sqrt{13}]. \end{aligned}$$

Now we have to partition edges of $D[n]$ for $n \geq 2$ on the basis of degrees of end vertices of every single edge.

$(d_u, d_v)$where $uv \in D[n]$	Number of edges
$(1,2)$	2^{t+1}
$(1,3)$	$4(2^t - 1)$
$(2,2)$	$10(2^{t+1}) - 26$
$(2,3)$	$7(2^{t+1}) - 8$

Table 3.2: For $n = 2t, t \geq 1$

$(d_u, d_v)$where $uv \in D[n]$	Number of edges
$(1,2)$	2^{t+1}
$(1,3)$	$4(2^t-1)$
(2,2)	$7(2^{t+2})-26$
(2,3)	$7(2^{t+1})-8$

Table 3.3: For $n = 2t+1, t \geq 1$

Here we have two cases

Case 1: when $n = 2t, t \geq 1$

Case 2: when $n = 2t+1, t \geq 1$

First we will calculate Sombor index of $D[n]$ for Case 1 :

$$\begin{aligned}
SO(D[n]) &= \sqrt{1^2+2^2}(2^{t+1}) + \sqrt{1^2+3^2}(4(2^t-1)) + \sqrt{2^2+2^2}(10(2^{t+1})-26) \\
&\quad + \sqrt{2^2+3^2}(7(2^{t+1})-8) \\
&= \sqrt{5}(2^{t+1}) + \sqrt{10}(4(2^t-1)) + \sqrt{8}(14(2^t-1)) + \sqrt{13}(7(2^{t+1})-8) \\
&= \sqrt{5}(2^{t+1}) + \sqrt{10}(4(2^t)) + \sqrt{8}(10(2^{t+1})) + \sqrt{13}(7(2^{t+1})) - \sqrt{10}(4) \\
&\quad - \sqrt{8}(26) - 8\sqrt{13} \\
&= \sqrt{5}(2^{t+1}) + \sqrt{10}(2(2^{t+1})) + \sqrt{8}(10(2^{t+1})) + \sqrt{13}(7(2^{t+1})) \\
&\quad - [\sqrt{10}\times 4 + \sqrt{8}\times 26 + 8\sqrt{13}] \\
&= 2^{t+1}[\sqrt{5} + 10\sqrt{8} + 2\sqrt{10} + 7\sqrt{13}] - [4\sqrt{10} + 26\sqrt{8} + 8\sqrt{13}].
\end{aligned}$$

Now we will calculate Sombor index of $D[n]$ for Case 2 :

$$\begin{aligned}
SO(D[n]) &= \sqrt{1^2+2^2}(2^{t+1}) + \sqrt{1^2+3^2}(4(2^t-1)) + \sqrt{2^2+2^2}(7(2^{t+2})-26) \\
&\quad + \sqrt{2^2+3^2}(7(2^{t+1})-8) \\
&= \sqrt{5}(2^{t+1}) + \sqrt{10}(4(2^t-1)) + \sqrt{8}(7(2^{t+2})-26) + \sqrt{13}(7(2^{t+1})-8) \\
&= \sqrt{5}(2^{t+1}) + \sqrt{10}(4(2^t)) - \sqrt{10}(4) + \sqrt{8}(7(2^{t+2}) - \sqrt{8}(26) + \sqrt{13}(7(2^{t+1})) - \sqrt{13}(8) \\
&= \sqrt{5}(2^{t+1}) + \sqrt{8}(7(2^{t+2})) + \sqrt{10}(4(2^t)) + \sqrt{13}(7(2^{t+1})) - 4\sqrt{10} - 26\sqrt{8} - 8\sqrt{13} \\
&= \sqrt{5}(2^{t+1}) + \sqrt{8}(7(2^{t+2})) + \sqrt{10}(2(2^{t+1})) + \sqrt{13}(7(2^{t+1})) - [4\sqrt{10} + 52\sqrt{2} + 8\sqrt{13}] \\
&= 2^{t+1}[\sqrt{5} + 14\sqrt{8} + 2\sqrt{10} + 7\sqrt{13}] - [4\sqrt{10} + 26\sqrt{8} + 8\sqrt{13}].
\end{aligned}$$

The proof is complete. □

3.2 Nanostar dendrimers $D_1[n]$

In this section, we will calculate Sombor index of nanostar dendrimer $D_1[n]$ as shown in Figure 3.2.

Theorem 3.2.1. *For graph of $D_1[n]$, the Sombor index is:*

$$D_1[n] = 24n\sqrt{2} + 12\sqrt{13}(2n-1) + 9\sqrt{2}(2n-1)$$

Proof. We know that formula of Sombor index is given as:

$$SO(D_1[n]) = \sum_{uv \in \xi(D[n])} \sqrt{{d_u}^2 + d_v^2}.$$

We are studying special class of Carbon nanostructures, that is, dendrimers which are

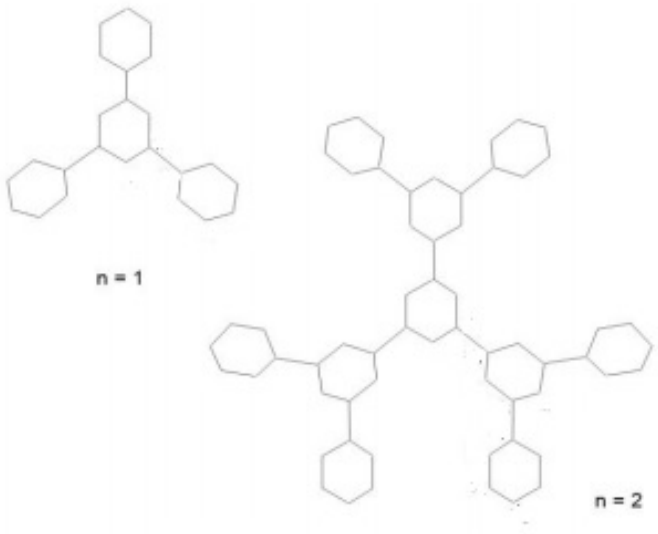


Figure 3.2: $D_1[n]$ with $n = 1$ and $n = 2$

basically important collection of molecular graphs so degree of vertices cannot exceed 4 therefore, let us consider

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

Then

$$SO(D[n]) = \sum_{(u,v)\in d} \sqrt{{d_u}^2 + d_v^2}\ m_{u,v} \tag{3.3}$$

where $m_{u,v}$ is the number of edges with end points u and v.

$$\begin{aligned} SO(D[n]) = {} & \sqrt{1^2+1^2}m_{1,1} + \sqrt{1^2+2^2}m_{1,2} + \sqrt{1^2+3^2}m_{1,3} + \sqrt{1^2+4^2}m_{1,4} \\ & + \sqrt{2^2+2^2}m_{2,2} + \sqrt{2^2+3^2}m_{2,3} + \sqrt{2^2+4^2}m_{2,4} + \sqrt{3^2+3^2}m_{3,3} \\ & + \sqrt{3^2+4^2}m_{3,4} + \sqrt{4^2+4^2}m_{4,4} \end{aligned}$$

It is clear from Figure 3.2 that all edges of $D_1[n]$ has degree coordinate of type $(2,2)$, $(2,3)$, $(3,3)$. Now we need to partition the edges on the basis of degrees of end vertices of every edge involved.

$(d_u, d_v)$where $uv \in D_1[n]$	Number of edges
$(2,2)$	$12n$
$(2,3)$	$12(2n-1)$
$(3,3)$	$3(2n-1)$

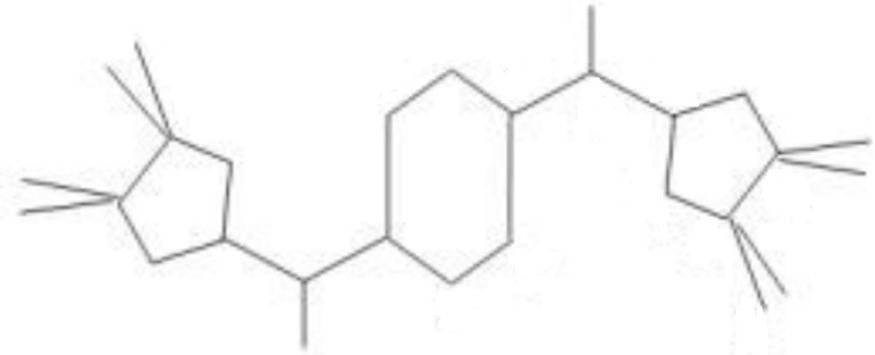
Table 3.4: Edge partition of $D_1[n]$ based on the degrees of end vertices of every single edge with $n \geq 1$

$$\begin{aligned}
SO(D[n]) &= \sqrt{1^2+1^2}(0) + \sqrt{1^2+2^2}(0) + \sqrt{1^2+3^2}(0) + \sqrt{1^2+4^2}(0) + \sqrt{2^2+2^2}(12n) \\
&+ \sqrt{2^2+3^2}(12(2n-1)) + \sqrt{2^2+4^2}(0) + \sqrt{3^2+3^2}(3(2n-1)) + \sqrt{3^2+4^2}(0) \\
&+ \sqrt{4^2+4^2}(0) \\
&= \sqrt{2^2+2^2}(12n) + \sqrt{2^2+3^2}(12(2n-1)) + \sqrt{3^2+3^2}(3(2n-1)) \\
&= \sqrt{8}(12n) + \sqrt{13}(12(2n-1)) + \sqrt{18}(3(2n-1)) \\
&= 24n\sqrt{2} + 12\sqrt{13}(2n-1) + 9\sqrt{2}(2n-1)
\end{aligned}$$

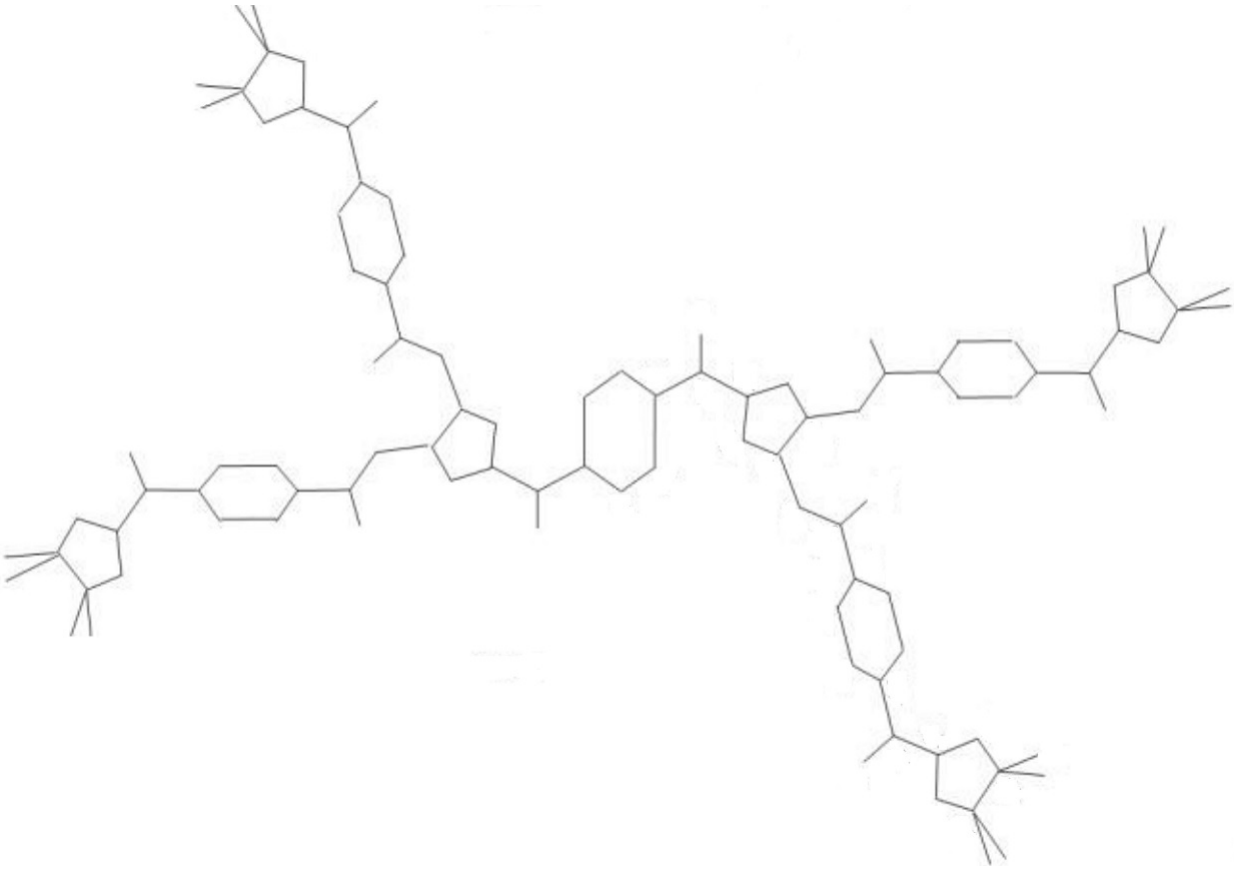
The proof is complete. □

3.3 Nanostar dendrimer $D_2[n]$

In this section we calculate the Sombor index of nanostar dendrimer $D_2[n]$ as shown in Figure 3.3.



(a) The graph of $D_2[n]$ with $n = 1$



(b) The graph of $D_2[n]$ with $n = 2$

Figure 3.3: Nanostar dendrimer $D_2[n]$ with $n = 1, 2$

Theorem 3.3.1. *For graph of $D_2[n]$, the Sombor index is*

$$SO(D_2[n]) = \begin{cases} (2^{n+2})[\sqrt{2}+\sqrt{5}+\sqrt{8}+4\sqrt{13}+\sqrt{10}+\sqrt{17}] & \\ +4\sqrt{13}(n^2-3n+2)+7(2^n)\sqrt{18}-2[15\sqrt{2}+3\sqrt{8} & \\ +3\sqrt{10}+10\sqrt{13}] & for\ n \geq 2 \\ 119.98 & for\ n = 1 \end{cases}$$

Proof. We know that formula of Sombor index is given as:

$$SO(D_2[n]) = \sum_{uv \in \xi(D_2[n])} \sqrt{{d_u}^2 + d_v^2}.$$

We are working on special type of molecular graphs where degree of vertices cannot exceed 4. Let

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

Then

$$SO(D_2[n]) = \sum_{(u,v) \in d} \sqrt{{d_u}^2 + d_v^2}\ m_{u,v} \tag{3.4}$$

where $m_{u,v}$ is the number of edges with end points u and v.

$$\begin{aligned} SO(D[n]) = {} & \sqrt{1^2+1^2}m_{1,1} + \sqrt{1^2+2^2}m_{1,2} + \sqrt{1^2+3^2}m_{1,3} + \sqrt{1^2+4^2}m_{1,4} \\ & + \sqrt{2^2+2^2}m_{2,2} + \sqrt{2^2+3^2}m_{2,3} + \sqrt{2^2+4^2}m_{2,4} + \sqrt{3^2+3^2}m_{3,3} \\ & + \sqrt{3^2+4^2}m_{3,4} + \sqrt{4^2+4^2}m_{4,4} \end{aligned}$$

First of all we need to partition the edges of $D_2[n]$ based upon degree of end vertices

of edges. Edge partition is shown in Table 3.6.

(d_u, d_v) where $uv \in D_2[n]$	Number of edges
$(1,3)$	$2^{n+2}-6$
$(1,4)$	$4(2^n)$
$(2,2)$	$2^{n+2}-6$
$(2,3)$	$4(n^2-3n+2)+2^{n+4}-20$
$(2,4)$	2^{n+1}
$(3,3)$	$14(2^{n-1})-10$
$(4,4)$	2^n

Table 3.5: Edge partition of $D_2[n]$ based on the degrees of end vertices of every single edge with $n \geq 2$

$$
\begin{aligned}
SO(D_2[n]) &= \sqrt{1^2+1^2}(0)+\sqrt{1^2+2^2}(0)+\sqrt{1^2+3^2}(2^{n+2}-6)+\sqrt{1^2+4^2}(4(2^n)) \\
&+ \sqrt{2^2+2^2}(2^{n+2}-6)+\sqrt{2^2+3^2}(4(n^2-3n+2)+2^{n+4}-20) \\
&+ \sqrt{2^2+4^2}(2^{n+1})+\sqrt{3^2+3^2}(14(2^{n-1})-10)+\sqrt{3^2+4^2}(0)+\sqrt{4^2+4^2}(2^n) \\
&= \sqrt{1^2+3^2}(2^{n+2}-6)+\sqrt{1^2+4^2}(4(2^n))+\sqrt{2^2+2^2}(2^{n+2}-6) \\
&+ \sqrt{2^2+3^2}(4(n^2-3n+2)+2^{n+4}-20)+\sqrt{2^2+4^2}(2^{n+1}) \\
&+ \sqrt{3^2+3^2}(14(2^{n-1})-10)+\sqrt{4^2+4^2}(2^n) \\
&= \sqrt{10}(2^{n+2}-6)+\sqrt{17}(4(2^n))+\sqrt{8}(2^{n+2}-6)+\sqrt{13}(4(n^2-3n+2)+2^{n+4}-20) \\
&+ \sqrt{20}(2^{n+1})+\sqrt{18}(14(2^{n-1})-10)+\sqrt{32}(2^n) \\
&= \sqrt{10}(2^{n+2})-\sqrt{10}(6)+\sqrt{17}(2^{n+2})+\sqrt{8}(2^{n+2})-\sqrt{8}(6)+\sqrt{13}(4(n^2-3n+2)) \\
&+ \sqrt{13}(2^{n+4})-\sqrt{13}(20)+\sqrt{5}(2^{n+2})+\sqrt{18}(7(2^n)-\sqrt{18}(10)+\sqrt{2}(2^{n+2}) \\
&= \sqrt{10}(2^{n+2})+\sqrt{17}(2^{n+2})+\sqrt{8}(2^{n+2})+4\sqrt{13}(2^{n+2})+\sqrt{5}(2^{n+2})+\sqrt{2}(2^{n+2}) \\
&+ \sqrt{13}(4(n^2-3n+2))+7\sqrt{18}(2^n)-\sqrt{10}(6)-\sqrt{8}(6)-\sqrt{13}(20)-\sqrt{18}(10)
\end{aligned}
$$

$$= (2^{n+2})[\sqrt{10} + \sqrt{17} + \sqrt{8} + 4\sqrt{13} + \sqrt{5} + \sqrt{2}] + 4\sqrt{13}(n^2 - 3n + 2) + 7\sqrt{18}(2^n)$$
$$- \sqrt{10}(6) - \sqrt{8}(6) - \sqrt{13}(20) - \sqrt{2}(30)$$
$$= (2^{n+2})[\sqrt{2} + \sqrt{5} + \sqrt{8} + 4\sqrt{13} + \sqrt{10} + \sqrt{17}] + 4\sqrt{13}(n^2 - 3n + 2) + 7(2^n)\sqrt{18}$$
$$- 6\sqrt{10} - 6\sqrt{8} - 20\sqrt{13} - 30\sqrt{2}$$
$$= (2^{n+2})[\sqrt{2} + \sqrt{5} + \sqrt{8} + 4\sqrt{13} + \sqrt{10} + \sqrt{17}] + 4\sqrt{13}(n^2 - 3n + 2) + 7(2^n)\sqrt{18}$$
$$- 2[15\sqrt{2} + 3\sqrt{8} + 3\sqrt{10} + 10\sqrt{13}]$$

The proof is complete. □

3.4 Hypercore dendrimer D_n

In this section we will calculate the Sombor index of hypercore dendrimer D_n as shown in Figure 3.4.

Theorem 3.4.1. *For graph of D_n, the Sombor index is*

$$SO(D_n) = (3\sqrt{10}+3\sqrt{17}+42\sqrt{2}+27\sqrt{13}+6\sqrt{5}+30)2^n-(2\sqrt{17}+30\sqrt{2}+15\sqrt{13}+6\sqrt{5}+15).$$

Proof. We know that formula of Sombor index is given as

$$SO(D_n) = \sum_{uv\in\xi(D_n)} \sqrt{{d_u}^2 + d_v^2}.$$

We can see from the Figure 3.4 that all the vertices of $D_2[n]$ has degree less than or equal to 4. Let

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

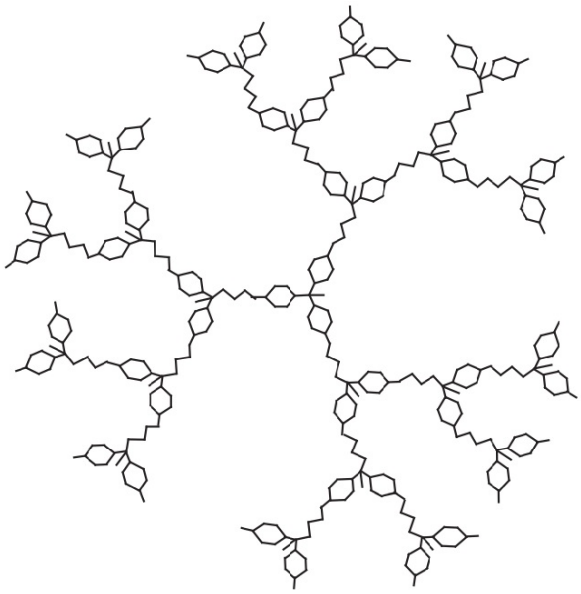


Figure 3.4: Hypercore dendrimer D_n with $n = 3$

Then

$$SO(D_n) = \sum_{(u,v)\in B} \sqrt{{d_u}^2 + d_v^2}\ m_{u,v}, \tag{3.5}$$

where $m_{u,v}$ is the number of edges with end points u and v.

$$\begin{aligned} SO(D_n) = {} & \sqrt{1^2+1^2}m_{1,1} + \sqrt{1^2+2^2}m_{1,2} + \sqrt{1^2+3^2}m_{1,3} + \sqrt{1^2+4^2}m_{1,4} \\ & + \sqrt{2^2+2^2}m_{2,2} + \sqrt{2^2+3^2}m_{2,3} + \sqrt{2^2+4^2}m_{2,4} + \sqrt{3^2+3^2}m_{3,3} \\ & + \sqrt{3^2+4^2}m_{3,4} + \sqrt{4^2+4^2}m_{4,4}. \end{aligned}$$

Edge partition of D_n based upon degree of end vertices $m_{u,v}$ is shown in Table 3.6, the size of D_n is equal to $63(2^n) - 38$.

(d_u, d_v) where $uv \in D_n$	Number of edges
$(1,3)$	$3(2^n)$
$(1,4)$	$3(2^n)-2$
$(2,2)$	$21(2^n)-15$
$(2,3)$	$27(2^n)-15$
$(2,4)$	$3(2^n)-3$
$(3,4)$	$6(2^n)-3$

Table 3.6: Edge partition of D_n based on the degrees of end vertices of every single edge

$$
\begin{aligned}
SO(D_n) &= \sqrt{1^2+1^2}\ \ (0) + \sqrt{1^2+2^2}\ \ (0) + \sqrt{1^2+3^2}\ \ (3(2^n)) + \sqrt{1^2+4^2}\ \ (3(2^n)-2) \\
&+ \sqrt{2^2+2^2}\ \ (21(2^n)-15) + \sqrt{2^2+3^2}\ \ (27(2^n)-15)) + \sqrt{2^2+4^2}\ \ (3(2^n)-3) \\
&+ \sqrt{3^2+3^2}\ \ (0) + \sqrt{3^2+4^2}\ \ (6(2^n)-3) + \sqrt{4^2+4^2}\ \ (0) \\
&= \sqrt{1^2+3^2}\ \ (3(2^n)) + \sqrt{1^2+4^2}\ \ (3(2^n)-2) + \sqrt{2^2+2^2}\ \ (21(2^n)-15) \\
&+ \sqrt{2^2+3^2}\ \ (27(2^n)-15)) + \sqrt{2^2+4^2}\ \ (3(2^n)-3) + \sqrt{3^2+4^2}\ \ (6(2^n)-3) \\
&= \sqrt{10}\ \ (3(2^n)) + \sqrt{17}\ \ (3(2^n)-2) + \sqrt{8}\ \ (21(2^n)-15) + \sqrt{13}\ \ (27(2^n)-15)) \\
&+ \sqrt{20}\ \ (3(2^n)-3) + \sqrt{25}\ \ (6(2^n)-3) \\
&= \sqrt{10}\ \ (3(2^n)) + \sqrt{17}\ \ (3(2^n)-2) + 2\sqrt{2}\ \ (21(2^n)-15) + \sqrt{13}\ \ (27(2^n)-15)) \\
&+ 2\sqrt{5}\ \ (3(2^n)-3) + 5\ \ (6(2^n)-3) \\
&= 3\sqrt{10}\ \ 2^n + 3\sqrt{17}\ \ 2^n + 42\sqrt{2}\ \ 2^n + 27\sqrt{13}\ \ 2^n + 6\sqrt{5}\ \ 2^n + 30\ \ (2^n) - 2\sqrt{17} \\
&- 30\sqrt{2} - 15\sqrt{13} - 6\sqrt{5} - 15 \\
&= (3\sqrt{10} + 3\sqrt{17} + 42\sqrt{2} + 27\sqrt{13} + 6\sqrt{5} + 30)2^n - 2\sqrt{17} - 30\sqrt{2} - 15\sqrt{13} \\
&- 6\sqrt{5} - 15 \\
&= (3\sqrt{10} + 3\sqrt{17} + 42\sqrt{2} + 27\sqrt{13} + 6\sqrt{5} + 30)2^n \\
&- (2\sqrt{17} + 30\sqrt{2} + 15\sqrt{13} + 6\sqrt{5} + 15)
\end{aligned}
$$

This proof is complete. □

Chapter 4

Silicate Structures

4.1 Silicate network $SLN(n)$

Silicate network can be constructed in many ways. Here we construct the silicate network from honey comb network. Let us consider a honey comb network $HCB(n)$ of n dimension. Now introduce silicon ions on all vertices of $HCB(n)$. Subdivide every edge of $HCB(n)$ for one time and place ion of oxygen on new generated vertices. Introduce new $6n$ pendent edges on each at silicon of degree 2 of $HCB(n)$. See Figure 4.1 . With each silicon ion connect the three ions of oxygen and form a tetrahedron, then the new network is called $SLN(n)$ as shown in Figure 4.2. In Figure 4.1 and 4.2 the graphs of silicon network are of dimension 2. The size and order of $SLN(n)$ is $36n^2$ and $15n^2 + 3n$, respectively.

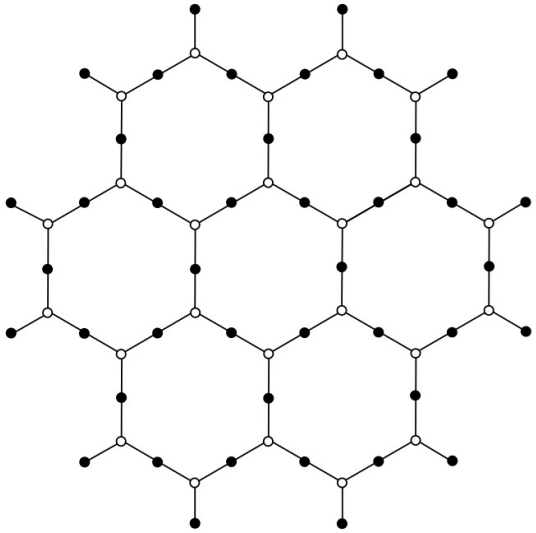


Figure 4.1: $HCB(n)$ to silicate network

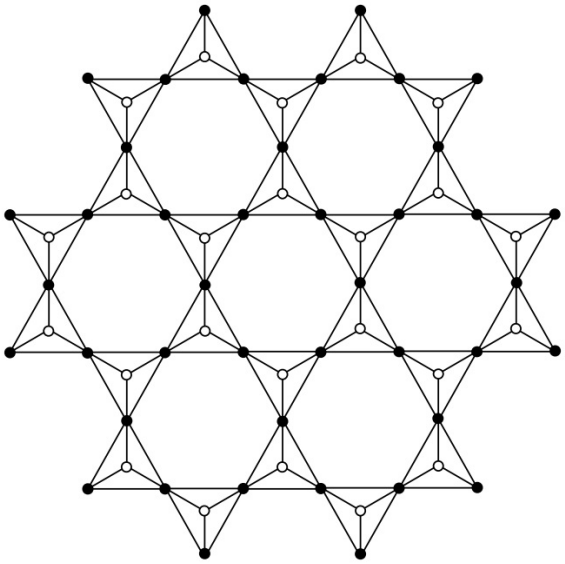


Figure 4.2: Construction of $HCB(n)$ to $SLN(n)$

Theorem 4.1.1. *The Somber index of $SLN(n)$ is given as*

$$SO(SLN(n)) = 54n\sqrt{2}\ \ (2n-1) + 18n\sqrt{5}\ \ (3n+1) \tag{4.1}$$

Proof. We know that formula of Sombor index is given as

$$SO(SLN(n)) = \sum_{uv \in \xi(SLN(n))} \sqrt{{d_u}^2 + d_v^2}.$$

It is clear from Figure 4.2 that all the vertices of $SLN(n)$ are of degree 3 or 6, so we need to partition the edges of $SLN(n)$ with respect to degree of vertices. All edges of $SLN(n)$ has d-coordinate $(3,3)$, $(3,6)$, $(6,6)$. [18] See Table 4.1.

(d_u, d_v) where $uv \in SLN(n)$	Number of edges
$(3,3)$	$6n$
$(3,6)$	$18n^2 + 6n$
$(6,6)$	$18n^2 - 12n$

Table 4.1: Edge partition of $SLN(n)$ based on the degrees of end vertices of every single edge.

Let

$$B = \{(3,3), (3,6), (6,6)\}$$

Then

$$SO(SLN(n)) = \sum_{uv \in B} \sqrt{{d_u}^2 + d_v^2} \;\; m_{u,v},$$

where $m_{u,v}$ is the number of edges with end points u and v.

$$\begin{aligned} SO(SLN(n)) &= \sqrt{3^2+3^2}m_{3,3} + \sqrt{3^2+6^2}m_{3,6} + \sqrt{6^2+6^2}m_{6,6} \\ &= \sqrt{3^2+3^2}(6n) + \sqrt{3^2+6^2}(18n^2+6n) + \sqrt{6^2+6^2} \;\; (18n^2-12n) \\ &= \sqrt{18}(6n) + \sqrt{45}(18n^2+6n) + \sqrt{72}(18n^2-12n) \\ &= 3\sqrt{2}(6n) + 3\sqrt{5}(18n^2+6n) + 6\sqrt{2}(18n^2-12n) \end{aligned}$$

$$= \sqrt{2}(18n) + 3\sqrt{5}(18n^2 + 6n) + \sqrt{2}(108n^2 - 72n)$$
$$= \sqrt{2}(18n + 108n^2 - 72n) + 3\sqrt{5}(18n^2 + 6n)$$
$$= \sqrt{2}(108n^2 - 54n) + 3\sqrt{5}(18n^2 + 6n)$$
$$= 54n\sqrt{2}(2n - 1) + 18n\sqrt{5}(3n + 1).$$

The proof is complete. □

4.2 Chain silicate network CS_n

Chain silicates are obtained by arranging tetrahedra linearly as shown in Fig. 4.3. It is denoted by (CS_n). The size and order of chain silicate network with $n > 1$ are $3n + 1$ and $6n$, respectively.

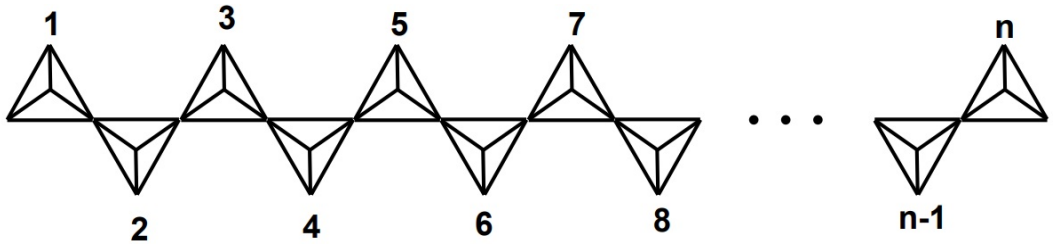


Figure 4.3: Chain silicate network of dimension n

Theorem 4.2.1. *The Sombor index of CS_n is given as:*

$$SO(CS_n) = 3(3\sqrt{2} + 4\sqrt{5})n - 6\sqrt{5} \tag{4.2}$$

Proof. We know that formula of Sombor index is given as

$$SO(CS_n) = \sum_{uv \in \xi(CS_n)} \sqrt{{d_u}^2 + d_v^2}.$$

Since, all edges of CS_n has *d-coordinate* $(3,3)$, $(3,6)$, $(6,6)$. So edge partition[18] of CS_n is shown in Table 4.2.

(d_u, d_v) where $uv \in CS_n$	Number of edges
$(3,3)$	$n+4$
$(3,6)$	$2(2n-1)$
$(6,6)$	$n-2$

Table 4.2: Edge partition of CS_n based on the degrees of end vertices of every single edge.

Let

$$B = \{(3,3),(3,6),(6,6)\}$$

Then

$$SO(CS_n) = \sum_{uv \in B} \sqrt{{d_u}^2 + d_v^2}\ \ m_{u,v},$$

where $m_{u,v}$ is the total number of edges with end points u and v.

$$\begin{aligned}
SO(CS_n) &= \sqrt{3^2+3^2}m_{3,3} + \sqrt{3^2+6^2}m_{3,6} + \sqrt{6^2+6^2}m_{6,6} \\
&= \sqrt{18}(n+4) + \sqrt{45}(2(2n-1)) + \sqrt{72}(n-2) \\
&= 3\sqrt{2}(n+4) + 3\sqrt{5}(4n-2)) + 6\sqrt{2}(n-2) \\
&= 3\sqrt{2}n + 12\sqrt{5}n + 6\sqrt{2}n + 12\sqrt{2} - 6\sqrt{5} - 12\sqrt{2} \\
&= 3\sqrt{2}n + 12\sqrt{5}n + 6\sqrt{2}n - 6\sqrt{5} \\
&= (3\sqrt{2} + 12\sqrt{5} + 6\sqrt{2})n - 6\sqrt{5} \\
&= (9\sqrt{2} + 12\sqrt{5})n - 6\sqrt{5} \\
&= 3(3\sqrt{2} + 4\sqrt{5})n - 6\sqrt{5}
\end{aligned}$$

The proof is complete. □

Bibliography

[1] Abdo, H., Dimitrov, D., Gutman, I. (2019). Graph irregularity and its measures. Appl. Math. Comput, 357, 317-324.

[2] Albertson, M. O. (1997). The irregularity of a graph. Ars Comb., 46, 219-225.

[3] Ali, A., Gutman, I., Milovanovic, E., Milovanovic, I. (2018). Sum of powers of the degrees of graphs: extremal results and bounds, MATCH Commun. Math. Comput. Chem, 80(1), 5-84.

[4] Cruz, R., Gutman, I., Rada, J. (2021). Sombor index of chemical graphs, Appl. Math. Comput., 399, 126018.

[5] Cruz, R., Rada, J. (2021). Extremal values of the Sombor index in unicyclic and bicyclic graphs, J. Math. Chem, 59(4), 1098-1116.

[6] Das, K. C., Çevik, A. S., Cangul, I. N., Shang, Y. (2021). On Sombor index. Symmetry, 13(1), 140.

[7] Deng, H., Tang, Z., Wu, R. (2021). Molecular trees with extremal values of Sombor indices, Int. J. Quantum Chem, 121(11), e26622.

[8] Furtula, B., Gutman, I. (2015). A forgotten topological index, J. Math. Chem, 53(4), 1184-1190.

[9] Favaron, O., Mahéo, M., Saclé, J. F. (1993). Some eigenvalue properties in graphs (conjectures of Graffiti—II), Discrete Math, 111(1-3), 197-220.

[10] Gutman, I., Furtula, B., Elphick, C. (2014). Three new/old vertex-degree-based topological indices, MATCH Commun. Math. Comput. Chem, 72(3), 617-632.

[11] Gutman, I. (2021). Geometric approach to degree-based topological indices: Sombor indices, MATCH Commun. Math. Comput. Chem, 86(1), 11-16.

[12] Kirby, E. C., Mallion, R. B., Polla, P., Skrzynski, P. J. (2016). What Kirchhoff actually did concerning spanning trees in electrical networks and its relationship to modern graph-theoretical work. Croat. Chem. Acta, 89(4), 1-16.

[13] Kulli, V. R. (2018). Reduced second hyper-Zagreb index and its polynomial of certain silicate networks. J. Appl. math. Inform., 14, 11-16.

[14] Liu, H. (2021). Ordering chemical graphs by their Sombor indices, arXiv preprint arXiv:2103.05995.

[15] Li, X., Shi, Y. (2008). A survey on the Randic index, MATCH Commun. Math. Comput. Chem, 59(1), 127-156.

[16] Lin, Z. (2021). On the spectral radius, energy and Estrada index of the Sombor matrix of graphs, arXiv preprint arXiv:2102.03960.

[17] Randic, M. (1975). Characterization of molecular branching, J. Am. Chem. Soc, 97(23), 6609-6615.

[18] Randić, M. (2004). Nenad Trinajstić–pioneer of chemical graph theory. Croat. Chem. Acta., 77(1-2), 1-15.

[19] Redžepović, I. (2021). Chemical applicability of Sombor indices: Survey, J. Serb. Chem. Soc, 86(5), 445-457.

[20] Réti, T., Došlic, T., Ali, A. (2021). On the Sombor index of graphs, Contrib. Math, 3, 11-18.

[21] Réti, T., Tóth-Laufer, E. (2017). On the construction and comparison of graph irregularity indices, Kragujev. J. Sci, (39), 53-75.

[22] Vasudev, C. (2006). Graph theory with applications. New Age International.

[23] Vukičević, D., Gašperov, M. (2010). Bond additive modeling 1, Adriatic indices. Croat. Chem. Acta, 83(3), 243-260.

[24] Wang, Z., Mao, Y., Li, Y., Furtula, B. (2021). On relations between Sombor and other degree-based indices, J. Appl. Math. Comput, 1-17.

[25] Wilson, R. J. (2004). History of graph theory. Section, 1, 29-49.

[26] Zhou, T., Lin, Z., Miao, L. (2021). The Sombor index of trees and unicyclic graphs with given maximum degree, arXiv preprint arXiv:2103.07947.