Extremal Graphs w.r.t Non-self-centrality Number

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MASTER'S THESIS WORK

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Dedication

This thesis is dedicated to my father for his endless support and encouragement.

Acknowledgement

All praises are for Almighty Allah, the most gracious and the most merciful, Who created this entire universe. I am highly grateful to Him for showering His countless blessings upon me and giving me the ability and strength to complete this thesis successfully and blessing me more than I deserve.

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Abstract

A topological index is a graph invariant that characterizes a molecular compound's topology. It is a type of molecular descriptor determined from a graph of a molecular compound. Recently, because of their growing range in the field of chemistry, topological indices have gained more significance.

Non-self-centrality (NSC) number is a graphical invariant which measures the non-self-centrality graphs. Earlier the upper and lower bounds on NSC number have been calculated and the graphs on which these bounds are attained have also been characterized. In this thesis we computed the NSC number of some nanotubes. We also determined trees with largest NSC number in the class of maximum fixed degree trees.

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Chapter 1

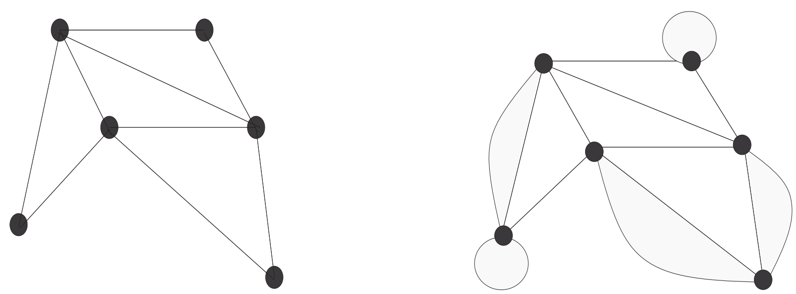
Introduction to Graph Theory

Recently, graph theory has become a significant mathematical tool in a variety of subjects such as; biology, chemistry, applied mathematics, commutative algebra, optimization theory, electrical engineering, bio-informatics, computer science, sociology, economics etc. The fundamental quality of graph theory is the connectivity in a system. This chapter contains basic concepts of graph theory that will be used later throughout this dissertation.

1.1 What is a graph?

A graph $\mathcal{G}$ is a representation of set of points and how they are connected. It is an ordered pair $(\mathcal{V}_\mathcal{G}, \mathcal{E}_\mathcal{G})$, where $\mathcal{V}_\mathcal{G}$ is a set of vertices and it is non-empty while, $\mathcal{E}_\mathcal{G}$ is a set of edges. There are two main classes of graphs; directed and undirected graphs. Throughout this dissertation graphs will be undirected.

Moreover, the number of elements in $\mathcal{V}_\mathcal{G}$ and $\mathcal{E}_\mathcal{G}$ is the order and size of $\mathcal{G}$, respectively. If the vertices $w, z \in \mathcal{V}_\mathcal{G}$ have an edge, $\{w, z\} \in \mathcal{E}_\mathcal{G}$, between them then w and z are adjacent in $\mathcal{G}$. For simplicity we denote an edge $\{w, z\}$ by wz or zw. The edge e is incident on w and z in $\mathcal{G}$ if $e = wz$. Also, w and z are the endpoints of e. If $e = ww$ for some $w \in \mathcal{V}_\mathcal{G}$ then e is a loop in $\mathcal{G}$. Furthermore, two edges $e_1, e_2 \in \mathcal{E}_\mathcal{G}$ are said to be multiple or parallel edges if $e_1 = wz = e_2$ for some $w, z \in \mathcal{V}_\mathcal{G}$. A graph $\mathcal{G}$ is called simple if it has no multiple edges and no loops otherwise; it is known as a multigraph. If we can find a path between every two distinct vertices of $\mathcal{G}$ then $\mathcal{G}$ is connected; otherwise $\mathcal{G}$ is disconnected. If a graph is disconnected then we say that the graphs has at least two components. A maximal connected subgraph of $\mathcal{G}$ is known as its component.



(a) (b)

Figure 1.1: (a) Simple graph. (b) Multigraph

1.2 Preliminaries

This section includes basic terminologies of graph theory.

Definition 1.2.1. The vertex degree $deg(z)$ of a vertex $z \in \mathcal{V}_\mathcal{G}$ is the number of edges incident with z.

Every edge adds 1 to the vertex degree of its end points while a loop contributes 2 to its end vertex. If $deg(z) = 1$, for some $z \in \mathcal{V}_\mathcal{G}$, then z is a pendant vertex of $\mathcal{G}$, while a vertex with $deg(z) = 0$ is known as isolated vertex.

Definition 1.2.2. For $w \in \mathcal{V}_\mathcal{G}$ the neighborhood $\mathcal{N}_w$ is defined as $\mathcal{N}_w = \{a \in \mathcal{V}_\mathcal{G} \mid aw \in \mathcal{E}_\mathcal{G}\}$.

We can define degree in terms of neighborhood, that is, for any $w \in \mathcal{V}_\mathcal{G}$ $deg(w) = |\mathcal{N}_w|$. If $|\mathcal{N}_w| = 0$ then w is known as isolated vertex. Similarly, if $|\mathcal{N}_w| = 1$ then w is a pendant vertex.

Definition 1.2.3. The minimum degree, denoted by $\delta_{\mathcal{G}}$, of $\mathcal{G}$ is the smallest degree of a vertex amongst all vertices of $\mathcal{G}$.

Definition 1.2.4. The maximum degree, denoted by $\Delta_{\mathcal{G}}$, of $\mathcal{G}$ is the largest degree of a vertex amongst all of $\mathcal{G}$.

From the Definitions 1.2.3 and 1.2.4, we can deduce that if $w \in \mathcal{V}_{\mathcal{G}}$ then $\delta \leq deg(w) \leq \Delta$. The graph is known as regular graph if $\delta_{\mathcal{G}} = \Delta_{\mathcal{G}}$.

In graph theory, a famous result by Leonhard Euler(1736) on the sum of degrees $\mathcal{G}$ is stated as follows:

Theorem 1.2.1 (The Handshaking Lemma)**.** *Consider a $\mathcal{G}$ of size m. Then*

$$2m = \sum_{w \in \mathcal{V}_{\mathcal{G}}} deg(w).$$

The above theorem is also called degree-sum formula. It shows that number of odd degree vertices is always even.

Definition 1.2.5. Consider a graph $\mathcal{G}$ and let $w, z \in \mathcal{V}_{\mathcal{G}}$. A path that connects w and z is the sequence of vertices $w = w_1, w_2, \ldots, w_k = z$, where for any $1 \leq i \leq (k-1)$, $w_i w_{i+1} \in \mathcal{E}_{\mathcal{G}}$ and $w_i \neq w_j$ for each i, j. Total edges in a path is the path length.

Definition 1.2.6. A sequence of vertices $C = \{w = w_1, w_2, \ldots, w_k = w\}$ such that $k \geq 3$, $w_i w_{i+1} \in \mathcal{E}_{\mathcal{G}}$ and $w_i \neq w_j$ for all i, j with $2 \leq i, j \leq (k-1)$ forms a cycle.

Girth (resp. circumference) of a graph is the length of smallest (resp. largest) cycle in a graph. A graph containing no cycle is called acyclic and the girth of an acyclic graph is defined to be infinite.

A graph $\mathcal{G}$ is complete if there is an edge between each two distinct vertices of $\mathcal{G}$ and it has largest size amongst all simple graphs. A complete graph of order q is denoted by K_q.

Definition 1.2.7. A set of pairwise adjacent vertices in $\mathcal{G}$ is called clique of $\mathcal{G}$.

In other words, we can define clique as a complete graph contained in $\mathcal{G}$. The set with largest size among all the cliques of $\mathcal{G}$ is the largest clique of $\mathcal{G}$. Clique number, $\omega_{\mathcal{G}}$, is the cardinality of a largest clique.

Definition 1.2.8. An independent set of a graph $\mathcal{G}$ is the set of pairwise non-adjacent vertices in $\mathcal{G}$.

If the vertex set $\mathcal{V}_{\mathcal{G}}$ of $\mathcal{G}$ is written as the union of two independent sets then, $\mathcal{G}$ is called a bipartite graph. Also, the independent sets are called partite sets of $\mathcal{G}$. Let $\mathcal{V}_{\mathcal{G}}^1$ and $\mathcal{V}_{\mathcal{G}}^2$ be two partite sets of a bipartite graph of order s. If each vertex in $\mathcal{V}_{\mathcal{G}}^1$ is connected to every vertex of $\mathcal{V}_{\mathcal{G}}^2$ then the graph is complete bipartite (a bi-clique) and is denoted by $K_{p,q}$, where $|\mathcal{V}_{\mathcal{G}}^1|= p$ and $|\mathcal{V}_{\mathcal{G}}^2|= q$. Also, $p + q = s$.

1.2.1 Subgraphs and isomorphic graphs

Definition 1.2.9. Let $\mathcal{G}$ be a graph. A graph $\mathcal{S} = (\mathcal{V}_{\mathcal{H}}, \mathcal{E}_{\mathcal{H}})$ is a subgraph of $\mathcal{G}$ if $\mathcal{E}_{\mathcal{S}} \subseteq \mathcal{E}_{\mathcal{G}}$ and $\mathcal{V}_{\mathcal{S}} \subseteq \mathcal{V}_{\mathcal{G}}$. We denote it as $\mathcal{S} \subseteq \mathcal{G}$.

A graph $\mathcal{S}$ is said to be an induced subgraph of $\mathcal{G}$ if $D \subseteq \mathcal{V}_{\mathcal{G}}$ is the set of vertices of $\mathcal{S}$ and contains edges of $\mathcal{G}$ with endpoints in D. Moreover, $\mathcal{S}$ is called spanning subgraph if $\mathcal{V}_{\mathcal{G}} = \mathcal{V}_{\mathcal{S}}$.

Definition 1.2.10. The graphs $\mathcal{G}$ and $\mathcal{H}$ are said to be isomorphic if there exists a bijective mapping $\gamma : \mathcal{V}_{\mathcal{G}} \longrightarrow \mathcal{V}_{\mathcal{H}}$ such that $w, z \in \mathcal{V}_{\mathcal{G}}$ are adjacent in $\mathcal{G}$ if and only if $\gamma(w)$ and $\gamma(z)$ are adjacent in $\mathcal{H}$. It is written as $\mathcal{G} \cong \mathcal{H}$.

An isomorphism [5] is an equivalence relation and partitions different classes of the graphs into equivalence classes.

1.2.2 Graph operations

Let $\mathcal{G}$ be a graph with $A \subseteq \mathcal{V}_{\mathcal{G}}$. Then the graph $\mathcal{G} - A$ is a vertex-deleted subgraph of $\mathcal{G}$ whose vertex set is $\mathcal{V}_{\mathcal{G}}$ and it contains those edges whose both ends are in $\mathcal{V}_{\mathcal{G}} - A$. If $\mathcal{G} - A$ disconnects $\mathcal{G}$ then, A is known as vertex cut. Moreover, a vertex $w \in \mathcal{V}_{\mathcal{G}}$ is a cut-vertex of $\mathcal{G}$ if $\mathcal{G} - w$ increases the components of $\mathcal{G}$. Also, let $S \subset \mathcal{V}_{\mathcal{G}}$. If for all $e \in \mathcal{E}_{\mathcal{G}}$, e has at least one endpoint in S then S is said to be the vertex cover of $\mathcal{G}$. Now let $Y \subseteq \mathcal{E}_{\mathcal{G}}$. Then the graph $\mathcal{G} - Y$ is an edge-deleted subgraph of $\mathcal{G}$ whose vertex set is $\mathcal{V}_{\mathcal{G}}$ and edge set is $\mathcal{E}_{\mathcal{G}} - Y$. If $\mathcal{G} - Y$ disconnects $\mathcal{G}$ then Y is said to be edge cut of $\mathcal{G}$. Also, a bridge or cut edge can be defined as an edge $e \in \mathcal{E}_{\mathcal{G}}$ such that $\mathcal{G} - e$ increases the components of $\mathcal{G}$. Furthermore, if $R \subset \mathcal{E}_{\mathcal{G}}$ then R is said to be the edge cover of $\mathcal{G}$ if every $w \in \mathcal{V}_{\mathcal{G}}$ is an end vertex of at least one edge in R.

For a simple graph $\mathcal{G}$, $\overline{\mathcal{G}}$ is complement of $\mathcal{G}$ if and only if $\mathcal{V}_{\mathcal{G}} = \mathcal{V}_{\overline{\mathcal{G}}}$ and $wz \in \mathcal{E}_{\overline{\mathcal{G}}} \iff wz \notin \mathcal{E}_{\mathcal{G}}$. A graph is said to be self-complementary if it is isomorphic to its complement.

Let $\mathcal{G}$ and $\mathcal{H}$ be vertex-disjoint graphs. The union of $\mathcal{G}$ and $\mathcal{H}$ is a graph whose vertex and edge sets are defined as $\mathcal{V}_{\mathcal{G}} \cup \mathcal{V}_{\mathcal{H}}$ and $\mathcal{E}_{\mathcal{G}} \cup \mathcal{E}_{\mathcal{H}}$, respectively. It is denoted by $\mathcal{G} \cup \mathcal{H}$. Similarly, the intersection is a graph with edge set $\mathcal{E}_{\mathcal{G}} \cap \mathcal{E}_{\mathcal{H}}$ and vertex set $\mathcal{V}_{\mathcal{G}} \cap \mathcal{V}_{\mathcal{H}}$. It is denoted by $\mathcal{G} \cap \mathcal{H}$

1.2.3 Distance and connectivity

Distance between $w, z \in \mathcal{V}_{\mathcal{G}}$ is the length of a shortest path between w and z. It is denoted by $d_{\mathcal{G}}(w, z)$. Whereas, eccentricity of a vertex $w \in \mathcal{V}_{\mathcal{G}}$ is defined as the largest distance between w and any other vertex of $\mathcal{G}$, that is,

$$e_{\mathcal{G}}(w) = \max_{z \in \mathcal{V}_{\mathcal{G}}} d_{\mathcal{G}}(w, z).$$

Definition 1.2.11. Diameter of a graph $\mathcal{G}$ is defined as the maximum eccentricity of a vertex in $\mathcal{G}$. It is denoted by $d(\mathcal{G})$. The vertex with maximum eccentricity is called peripheral vertex of $\mathcal{G}$.

Definition 1.2.12. Radius of a graph $\mathcal{G}$ is defined as the minimum eccentricity of a vertex in $\mathcal{G}$. It is denoted by $r(\mathcal{G})$. The vertex with minimum eccentricity is called the central vertex of the graph $\mathcal{G}$.

If $d(\mathcal{G}) = r(\mathcal{G})$ then $\mathcal{G}$ is called a self-centered graph; otherwise, $\mathcal{G}$ is known as a non-self-centered graph.

If $\mathcal{G}$ remains connected by deleting q vertices then $\mathcal{G}$ is q-connected. Similarly, $\mathcal{G}$ is q-edge-connected whenever $\mathcal{G}$ remains connected by deleting q edges.

An n by n symmetric matrix of an n-vertex graph $\mathcal{G}$ is called adjacency matrix $A_{\mathcal{G}} = [a_{ij}]_{n\times n}$ of $\mathcal{G}$ if

$$a_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in \mathcal{E}_{\mathcal{G}} \\ 0 & \text{otherwise.} \end{cases} \tag{1.1}$$

Incidence martix $M_{\mathcal{G}} = [m_{ij}]_{n\times m}$ of a graph $\mathcal{G}$ is defined by

$$m_{ij} = \begin{cases} 1 & \text{if } v_i \in \mathcal{V}_{\mathcal{G}} \text{ is an endpoint of } e_j \in \mathcal{E}_{\mathcal{G}} \\ 0 & \text{otherwise.} \end{cases} \tag{1.2}$$

A graph is singular if $A_{\mathcal{G}}$ is singular otherwise, $\mathcal{G}$ is said to be non-singular.

1.3 Matching and dominating set

For any graph $\mathcal{G}$, a subset of the edges such that no two edges in the subset share a vertex of $\mathcal{G}$ is called matching of $\mathcal{G}$ denoted by $M(\mathcal{G})$. A matching is said to be maximal if no more edges can be added to $M(\mathcal{G})$. Whereas, if $M(\mathcal{G})$ has the largest number of elements among all matchings of $\mathcal{G}$ then it is said to be a maximum matching. Moreover, matching number is the number of edges in a maximum matching. In a matching the vertex degree is either 0 or 1. Let $w \in \mathcal{V}_{\mathcal{G}}$ then w is called M-saturated if w is an endpoint of some edge in $M(\mathcal{G})$; otherwise unsaturated. Moreover, a matching is perfect if all vertices in $\mathcal{G}$ are M-saturated. Every perfect matching is maximum but the converse is not true. Let $\mathcal{A} \subset \mathcal{V}_{\mathcal{G}}$. Then $\mathcal{A}$ is said to be the dominating set of $\mathcal{G}$ when for all $z \in \mathcal{V}_{\mathcal{G}} \backslash \mathcal{A}$, z is adjacent to a vertex $w \in \mathcal{A}$.

1.4 Trees and related structures

A simple and connected graph having no loops or cycles is a tree. This mathematical structure was first studied by Cayley [9] in 1857. Furthermore, an n-vertex tree always has $n-1$ edges. In a tree, all edges are bridges since, there is exactly one path joining every two vertices. A pendant vertex of a tree is called leaf. A tree is either uni-central or bi-central. Also, a graph whose all components are trees is a forest.

A tree with maximum diameter 2 is known as a star. A star S_q, of order q has $(q-1)$ pendant vertices attached to a single vertex of degree $q-1$. A tree having a perfect matching is said to be a conjugated tree. Moreover,if there exists a path P in a tree T such that every vertex in $\mathcal{V}_T$ either belongs to P or is at a distance of one edge from P, then T is known as a caterpillar. A subgraph $\mathcal{S}$ of $\mathcal{G}$ is a spanning tree if it contains all the vertices of $\mathcal{G}$ and is a tree.

1.4.1 Extremal graph theory

A branch of graph theory which studies that how the properties of graphs such as size, order, edge density, chromatic number, girth, diameter and degree etc., influence the structures is known as Extremal graph theory. The main objective is to study the extremal graphs, which are either maximal or minimal with some fixed parameter. In 1907, Mantel [31] proved a theorem which gives the basic statement of extremal graph theory.

Theorem 1.4.1 (Mantel's Theorem [31]). *If an n-vertex graph $\mathcal{G}$ contains no triangle then it contains at most $\frac{n^2}{4}$ edges.*

In 1941, Paul Turan [42] worked for the advancement of extremal graph theory as he generalizes Mantel's theorem by using clique of size r.

Theorem 1.4.2 (Turan Theorem [42]). *If $\mathcal{G}$ is an n-vertex graph that contains no copy of K_{q+1}, the complete graph on $q+1$ vertices, then it contains at most $\left(1-\frac{1}{q}\right)\frac{n^2}{2}$ edges.*

Turan's theorem became the motivation for the later results in extremal graph theory, such as Erdős-Stone-Simonovits theorem in 1946. Erdős and Stone [15] also extended the Turan's theorem for the graphs that do not contain the complete multi-partite graphs.

Theorem 1.4.3 (Erdős-Stone-Simonovits Theorem [15]). *For given real number $\epsilon > 0$ and natural numbers r, s, there is an integer $b_0(r, s.\epsilon)$ such that if an n-vertex graph*

$\mathcal{G} = (\mathcal{V}_\mathcal{G}, \mathcal{E}_\mathcal{G})$ *with* $|\mathcal{V}_\mathcal{G}| > b_0(r, s, \epsilon)$ *and* $|\mathcal{E}_\mathcal{G}| > \frac{(1-\frac{1}{r}+\epsilon)|\mathcal{V}_\mathcal{G}|^2}{2}$ *then,* $\mathcal{G}$ *contains a complete* $(r+1)$*-partite graph.*

Identifying the extremal graphs in a given class of graphs with reference to a topological invariant has gained a significant importance in extremal graph theory. We have a number of excellent results in this area of graph theory. We can also see that same graphs can be obtained for certain classes of graphs.

Chapter 2

Chemical graph theory and topological invariants

A chemical graph is a convenient model for real and abstract chemical systems. Therefore, chemical graph theory can be categorized as the branch of mathematical chemistry that deals with the solution of the molecular problems by simply using the applications of graph theory. More than any other science, chemistry has made a sufficient use of the concepts of graph theory as formation and decomposition of bonds is an interesting topic for the chemists. The past two decades have witnessed a significant growth in the field of chemical graph theory. Chemical graphs were introduced in mathematical literature by Sylvester [40] and Cayley [9]. They used it for the purpose of representing and delineating chemical species by designing the structural formulas for the chemical graphs and then examining the similarities among them. Furthermore, graph theory has gained popularity in chemistry for many reasons. Firstly, no concept in natural sciences is as closely related to the structural formula of a compound than a graph. It appears that chemical graph theory provides a natural language for the chemists to communicate the concepts of chemistry. Secondly, graph theory gives easy rules to obtain qualitative predictions of different properties of compounds. Thirdly, graph theory can be used for the representation, classification, and categorization of chemical systems. Also, in this area graph theory is the most useful tool. The main goal of chemical graph theory is to reduce the molecular structure to a single number by using the algebraic invariant. The reduction of the molecule using the invariants gives energy of the molecule, structural fragments, its electronic structures or its molecular branching. A molecular graph $\mathcal{G}$ describes the structural formula of a chemical compound. The atoms are represented as vertices while, bonds between the atoms are edges of a graph $\mathcal{G}$. In this dissertation we are only concerned with the topological properties or topological invariants of a molecular compound. For the applications of topological indices, we refer the readers to [22, 27].

2.1 Topological indices

A topological index is a graph invariant [23, 21], which is a single number that characterizes the topology of a molecular compound. It is known as connectivity index. It is widely used in the fields of molecular topology, mathematical chemistry and chemical graph theory [3]. Topological indices are used in the development of QSPR and QSAR in which chemical structures are associated with biological or other properties of the molecules.

The study of topological indices started in 1947 by the introduction of Wiener index. It establishes the relationship between the physico-chemistry and the structures of the molecular graphs of alkenes. In present, there are more than 120 topological indices [6] and the fact they are still used today is that they are durable and versatile. Various studies show that there is a strong relationship between the chemical characteristics of drugs and chemical compounds such as, boiling points and melting points, and their structures. Therefore, researchers can understand the chemical reactivity, biological activity and physical features if they use topological indices defined on these molecular structures. Recently, the topological indices proves to be a feasible tool in studying the molecular structures of nanotubes, nanocones etc.

The topological indices are usually related to either connectivity, or graph theoretical (topological) distances in a graph $\mathcal{G}$. For further study on this topic, we refer the reader [36].

2.1.1 Connectivity based topological indices

The topological indices in this section either base on the sum of degrees of vertices or the graph spectrum of a graph.

The Zargeb indices

During the work on the topological basis of π-electron energy [19] of a conjugated system, the Zargeb group got two terms in the formula. These two terms can separately be used as two different topological indices [18]. The indices were named as first Zagreb index $M_{1_\mathcal{G}}$ and second Zagreb index $M_{2_\mathcal{G}}$ are given by

$$M_{1_\mathcal{G}} = \sum_{w \in \mathcal{V}_\mathcal{G}} (deg(w))^2, \tag{2.1}$$

$$M_{2_\mathcal{G}} = \sum_{wz \in \mathcal{E}_\mathcal{G}} deg(w)deg(z). \tag{2.2}$$

The sum in (2.1) is over all the vertices of $\mathcal{G}$ while the sum in (2.2) is over all the edges of $\mathcal{G}$.

The connectivity index

The connectivity index of a graph $\mathcal{G}$, similar to Zargeb group of indices, was introduced by Randic [35]. It is denoted by $\chi(\mathcal{G})$. Randic [35] defines connectivity index of a graph as bond additive quantity and it is widely used in QSPR and QARS.

$$\chi(\mathcal{G}) = \sum_{u_iu_j \in \mathcal{E}_\mathcal{G}} [deg(u_i)deg(u_j)]^{-1/2}. \tag{2.3}$$

Thus, $\chi(\mathcal{G})$ is the sum of bond weights given by $[deg(u_i)deg(u_j)]^{-1/2}$.

The connectivity ID number

This number was introduced by Randic [34]. The connectivity ID number is defined on connectivity wights and the path counts.
The connectivity weight $w(u_iu_j)$ where, $u_iu_j \in \mathcal{E}_\mathcal{G}$ is given by

$$w(u_iu_j) = [deg(u_i)deg(u_j)]^{-1/2}.$$

One can also use the weighted paths $w(q_t)$ instead of weighted edges, which is defined as

$$w(q_t) = \prod_{i=1}^{t} w(u_i u_{i+1}),$$

where q_t is the weighted path of length t and $u_i u_{i+1}$ is the set of weighted edges that form a path. Mathematically,

$$\mathrm{ID} \quad = \quad |\mathcal{V}_\mathcal{G}| + \frac{1}{2} \sum_{q_t} w(q_t). \tag{2.4}$$

The connectivity ID number is used effectively in various QSAR studies like classifying anticholinergic compounds. Apart from this, there is one problem with this index that is, enumeration of paths. This becomes an obstacle with the increase in the size of a molecular graph.

The Z-index

This index was introduced by Hosoya [23] and is defined as

$$Z(\mathcal{G}) \quad = \quad \sum_{h=0}^{[\mathcal{V}_\mathcal{G}/2]} a(\mathcal{G}; h), \tag{2.5}$$

where $a(\mathcal{G}; h)$ is the number of independent sets of h edges of $\mathcal{G}$. A set S of h edges is independent if no two edges of the set S are adjacent in $\mathcal{G}$. The empty set and all singleton sets are independent, hence $a(\mathcal{G}; 0) = 1$ and $a(\mathcal{G}; 1)$ equals the number of edges in $\mathcal{G}$.

2.1.2 Topological indices based on distances

Several early topological indices were based on distances. Some of them are discussed in this section.

The Wiener index

Wiener index was introduced in 1947 by Harold Wiener [46]. At the beginning it was known as path invariant but later it was named as Wiener index. Later, in 1971 its notion was defined by Hosoya [23] as

$$\mathcal{W}(\mathcal{G}) = \sum_{\{w,z\}\subseteq\mathcal{V}_{\mathcal{G}}} d_{\mathcal{G}}(w,z). \tag{2.6}$$

The implementations of the Wiener index can be seen in [13]. Another index introduced by Harold Wiener [46] is known as Wiener polarity index. It is described as the number of unordered pairs $\{w, z\}$ of vertices in $\mathcal{G}$ with $d_{\mathcal{G}}(w, z) = 3$. Mathematically,

$$\mathcal{W}_{\mathbf{p}}(\mathcal{G}) = |\{\{w,z\} \mid d_{\mathcal{G}}(w,z) = 3, \text{ for } u_i, u_j \in \mathcal{V}_{\mathcal{G}}\}|. \tag{2.7}$$

The chemical and mathematical applications of this index were later studied by Lukovits and Linert [30], and Hosoya [24].

Another old index which was introduced in the continuation of Wiener index is the hyper Wiener index. It was introduced by Randic [35]. Mathematically,

$$\mathcal{WW}(\mathcal{G}) = \frac{1}{2}\sum_{w\in\mathcal{V}_{\mathcal{G}}}\sum_{z\in\mathcal{V}_{\mathcal{G}}}\Big[d_{\mathcal{G}}(w,z) + (d_{\mathcal{G}}(w,z))^2\Big]. \tag{2.8}$$

The Platt number

The Platt number was introduced by Platt [32, 33] as he was interested in introducing the scheme for the physical parameters such as molar volumes, heat of formation, heat of vaporization etc. of alkanes. The Platt number is the total sum of edge-degrees in a graph $\mathcal{G}$. The edge-degree of $deg(w,z) = deg(e_i)$ of an edge $e_i \in \mathcal{E}_\mathcal{G}$ is the number of adjacent edges. Mathematically,

$$\mathcal{F}_\mathcal{G} = \sum_{i=1}^{M} deg(e_i). \tag{2.9}$$

The Gordon-Scantlebury index

The Gordon-Scantlebury index [16] of a graph $\mathcal{G}$ is denoted by $\mathcal{S}_\mathcal{G}$. It is defined as the number of all the paths $\mathcal{L}_3$, of length 2 in $\mathcal{G}$. Mathematically,

$$\mathcal{S}_\mathcal{G} = \sum_{i} (\mathcal{L}_3)_i \tag{2.10}$$

For the applications we refer reader to [16].

The Balaban number

This topological index was introduced by Balaban [4] based on the distance sum of vertices and cyclomatic number of the graph $\mathcal{G}$.

The distance sum $d_\mathcal{G}(w_i) = d_i$ is defined as the sum of distances of w_i from each vertex of $\mathcal{G}$. Whereas, cyclomatic number $\mu_\mathcal{G}$ of $\mathcal{G}$ is the least number of edges whose removal from $\mathcal{G}$ to converts it into an acyclic graph. The number $\mu_\mathcal{G} = |\mathcal{E}_\mathcal{G}| - |\mathcal{V}_\mathcal{G}| + 1$ is the cyclomatic number of policyclic graph.

Hence, the Balaban number $\mathcal{J}_\mathcal{G}$ is given by

$$\mathcal{J}_\mathcal{G} = \frac{|\mathcal{E}_\mathcal{G}|}{\mu(\mathcal{G}) + 1} \sum_{\{u_i, u_j\}} [d_i d_j]^{-1/2} \tag{2.11}$$

The centric index

Balaban [4] introduced an invariant which reflects the shape of alkanes. It was named as the centric index. The distance r_i between u_i and any other vertex u_j in $\mathcal{G}$ is defined as

$$r_i = \max_{u_j \in \mathcal{V}_\mathcal{G}} d_\mathcal{G}(u_i, u_j). \tag{2.12}$$

Then

$$r = \min_{u_j \in \mathcal{V}_\mathcal{G}} (d_\mathcal{G})(r_i) \tag{2.13}$$

is known as the radius of $\mathcal{G}$ and each vertex with $r = r_i$ is the central vertex of $\mathcal{G}$. Center of a graph $\mathcal{G}$ is the set of all central vertices of $\mathcal{G}$.

Many eccentricity based invariants and their implementations are introduced in mathematics and chemistry. Some of them are discussed here.

Average eccentricity index

Skorobogatov and Dobryninin [39] in 1988 brought the notion of average eccentricity index and it is defined as follows:

$$\bar{\epsilon}_\mathcal{G} = \frac{1}{|\mathcal{V}_\mathcal{G}|} \sum_{w_i \in \mathcal{V}_\mathcal{G}} e_\mathcal{G}(w_i). \tag{2.14}$$

For more results on average eccentricity index we refer readers to [14, 8, 41]

Eccentric connectivity invariant

Sharma et al. [38] introduced a degree and eccentricity based invariant known as eccentric connectivity index. Mathematically it is defined as

$$\xi^c_\mathcal{G} = \sum_{w_i \in \mathcal{V}_\mathcal{G}} e_\mathcal{G}(w_i) deg(w_i). \tag{2.15}$$

The eccentric connectivity index provides a high level of anticipatebility of pharmaceutical characteristics and allow directions of beneficial and protected anti-HIV compounds. The connection between the Wiener index and eccentric connectivity index is examined by Gupta et al.[17]. For the mathematical characteristics of this index one can see [26, 37, 54].

Connective eccentricity index

In the continuation of eccentric connectivity index Gupta et al. put forward another index named connective eccentricity index. It is denoted by $\xi^{ce}(\mathcal{G})$ and is illustrated as

$$\xi^{ce}_{\mathcal{G}} = \sum_{w_i \in \mathcal{V}_{\mathcal{G}}} \frac{deg(w_i)}{e_{\mathcal{G}}(w_i)}. \tag{2.16}$$

Eccentric adjacency index

Eccentric adjacency index is the variation of the eccentric connectivity index and the connective eccentricity index. Mathematically,

$$\xi^{ad}_{\mathcal{G}} = \sum_{w_i \in \mathcal{V}_{\mathcal{G}}} \frac{\mathcal{S}_{\mathcal{G}}(w_i)}{e_{\mathcal{G}(w_i)}}, \tag{2.17}$$

where $\mathcal{S}_{\mathcal{G}}(w_i)$ is the sum of degrees of linked vertices of $w_i \in \mathcal{V}_{\mathcal{G}}$ and is described as

$$\mathcal{S}_{\mathcal{G}}(u_i) = \sum_{w_j \in \mathcal{N}_{w_i}} deg(w_j).$$

Total eccentricity index

Total eccentricity index is another topological index that is derived from eccentric connectivity index. It is illustrated as

$$\tau(\mathcal{G}) = \sum_{u_i \in \mathcal{V}_{\mathcal{G}}} e_{\mathcal{G}}(u_i). \tag{2.18}$$

Zagreb eccentricity indices

In previous section we have seen that the Zagreb group indices [19] are defined in terms of degree but were later expressed in terms of eccentricity. Vukicevic and Graovac [44] defined them as follows

$$M_1(\mathcal{G}) = \sum_{u_i \in \mathcal{V}_{\mathcal{G}}} [e_{\mathcal{G}}(u_i)]^2, \tag{2.19}$$

and

$$M_2(\mathcal{G}) = \sum_{u_i u_j \in \mathcal{E}_\mathcal{G}} e_\mathcal{G}(u_i) e_\mathcal{G}(u_j). \tag{2.20}$$

Furthermore, the third Zargeb index [51] is also introduced and is defined as

$$M_3(\mathcal{G}) \;\; = \;\; \sum_{u_i u_j \in \mathcal{E}_\mathcal{G}} |e_j - e_i|. \tag{2.21}$$

The third Zagreb index is a good indicator of non-self-centrality of a graph $\mathcal{G}$.

Non-self-centrality number

After third Zagreb index, non-self-centrality number [51] is introduced for better indication of non-self-centrality $\eta(\mathcal{G})$ of a graph $\mathcal{G}$. Mathematically,

$$\eta(\mathcal{G}) \;\; = \;\; \sum_{u_i \neq u_j} |e_j - e_i|, \tag{2.22}$$

where the summation is over all the unordered pairs in $\mathcal{G}$.
The non-self-centrality number can be restated in terms of the eccentricity sequence. For a graph $\mathcal{G}$ the eccentricity sequence $\zeta(\mathcal{G})$ is the set of distinct eccentricities in $\mathcal{G}$ with their multiplicities. Assume that $e_1 > e_2 > \cdots > e_k$ be k distinct eccentricities of $\mathcal{G}$ with their respective multiplicities $l_1, l_2, \ldots, l_k$. Then we have

$$\eta(\mathcal{G}) \;\; = \;\; \sum_{1 \leq i < j \leq k} l_i l_j (e_i - e_j). \tag{2.23}$$

Chapter 3

Non-self-centrality number of some molecular graphs

In this chapter we consider some molecular graphs, that is TUC_4C_8 and V-phynelenic nanotubes. We calculate the NSC number of these graphs. Furthermore, we calculate the NSC number of TUC_4C_8 and V-phynelenic nanotori.

3.1 V-Phynelenic nanotubes

Here we compute the non-self centrality number of V-Phynelenic nanotubes. An infinte structure of V-Phynelenic nanotubes and nanotori is made by alternating C_4, C_6 and C_8 cycles. The arrangement of C_4, C_6 and C_8 cycles in V-Phynelenic structure is such that C_4 ring is attached to two C_6 rings and also each C_4 is attached to two C_8 rings. We will denote the V-Phynelenic nanotubes by $T[h, f]$, where f and h are the number of columns and rows, respectively, as shown in the Figure 3.1 and 3.2. Consider

$$X = \{z \in \mathcal{V}(T[h, f]) \mid \deg(z) = 2\},$$

$$Y = \{z \in \mathcal{V}(T[h, f]) \mid \deg(z) = 3\}.$$

Then $|X|= 2h$ and $|Y|= 6hf - 2h$. From the structure of $T[h, f]$, we notice that there are two types of edges given by

$$\mathcal{E}_1 = \{wz \in \mathcal{V}(T[h, f]) \mid \deg(w), \deg(z) = (2, 3)\}$$

and

$$\mathcal{E}_2 = \{wz \in \mathcal{V}(T[h,f]) \mid (\deg(w), \deg(z)) = (3,3)\}.$$

It is easy to see that $|\mathcal{E}_1| = 4h$ and $|\mathcal{E}_2| = h(9f-5)$. Hence, $|\mathcal{E}| = |\mathcal{E}_1| + |\mathcal{E}_2| = h(9f-1)$ is the number of total edges in $T[h,f]$.

Before moving to the main results, it is important to know that structure of V-Phynelenic nanotube is symmetric and hence it can be divided into two halves as shown in Figure 3.1. Whereas, we can also divide the structure into two different classes depending on h and f. When $h < 2f$ we get a vertical structure shown in Figure 3.2, while we obtain a horizontal structure for $h > 2f$. Now let us begin with the following result:

Lemma 3.1.1. *For $f \geq 2$ the diameter of $T[h,f]$ is*

$$d(T[h,f]) = \begin{cases} \frac{h}{2} + 4f - 1 & h \leq 2f \text{ and } h \text{ is even} \\ \frac{h-3}{2} + 4f & \text{if } h \leq 2f \text{ and } h \text{ is odd} \\ \frac{3h}{2} + 2f - 1 & \text{if } h > 2f \text{ and } h \text{ is even} \\ \frac{3(h-1)}{2} + 2f & \text{if } h > 2f \text{ and } h \text{ is odd.} \end{cases} \tag{3.1}$$

Proof. Let w_i and z_j, $1 \leq i,j \leq h$, be the peripheral vertices in $T[h,f]$, as shown in Figure 3.1. We can partition $\mathcal{E}(T[h,f])$ into three classes; horizontal, oblique and vertical edges. Now if $h \leq 2f$ and h is an even integer then, to find the diameter we have to find the path's length that connects two vertices of X. Let w_i be the vertex with an eccentric vertex z_j in $T[h,f]$, shown in Figure 3.1. For $j < (\frac{h}{2} + i)$, length of a shortest w_i, z_j-path contains $2f$ oblique, $(2f-1)$ vertical and $j-1$ horizontal edges. Therefore,

$$d_{T[h,f]}(w_i, z_j) = 4f + j - 2.$$

Similarly, for $j = (\frac{h}{2} + i)$, the length of a shortest w_i, z_j-path contains exactly $2f-1$ vertical, $2f$ oblique and $\frac{h}{2}$ horizontal edges. Therefore,

$$d_{T[h,f]}(w_i, z_j) = \frac{h}{2} + 4f - 1.$$

Now for $j > (\frac{h}{2} + i)$, the length of the shortest w_i, z_j-path contains $2f$ oblique, $(2f-1)$ vertical and $h - j$ horizontal edges. Therefore,

$$d_{T[h,f]}(w_i, z_j) = 4f + h - j.$$

From the above discussion and Figure 3.1, it is observed that $d_{T[h,f]}(w_i, z_j) = \frac{h}{2} + 4f - 1$ is the maximum distance of therefore, $d(T[h, f]) = \frac{h}{2} + 4f - 1$.

Similarly, in case of odd h, we choose w_i and z_j, where $z_j \in X \cup Y$, such that $d_{T[h,f]}(w_i, z_j)$ is maximum. We need $2f$ oblique edges, $2f - 1$ vertical edges and $\frac{h-1}{2}$ horizontal edges to connect w_i and z_j. Hence, the diameter is given by $d(T[h, f]) = \frac{h-3}{2} + 4f$. In similar manner, we can find the diameter of $T[h, f]$ when $h < 2f$. □

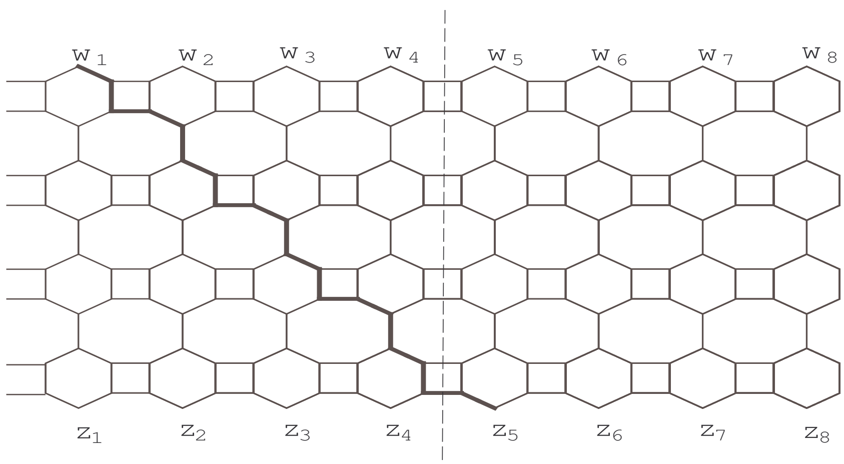


Figure 3.1: $T[8, 4]$

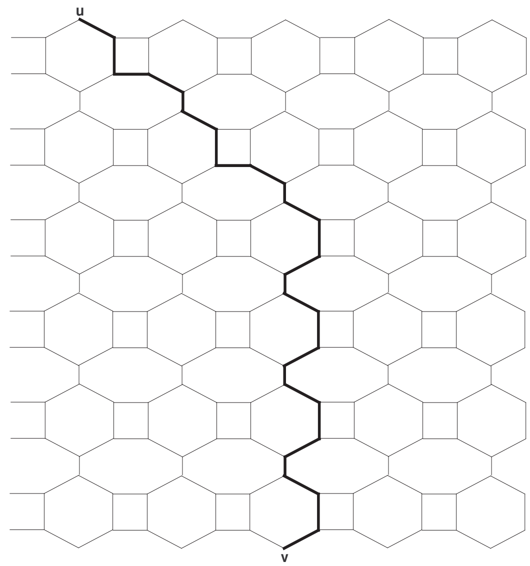


Figure 3.2: $T[5,6]$

Theorem 3.1.1. *For $f \geq 2$, we have*

$$\eta(T[h,f]) = \begin{cases} 2h^2 f[3f^2+1] & \text{if } h > 2f-1 \\ & \text{and } h \text{ is even} \\ 6fh^2(f+1)(f-1) & \text{if } h > 2f-1 \\ & \text{and } h \text{ is odd} \\ h^2[6f^3+122f-216] & \text{if } h = 2f-2 \\ & \text{or } h = 2f-1 \\ 4h^2\left[2f^3+\frac{s}{2}(2f^2-5)\right] & \text{if } h < 2f-2 \\ & \text{and } f \text{ is even} \\ 4h^2[3f^3-f] & \text{if } h < 2f-2 \\ & \text{and } f \text{ is odd.} \end{cases} \qquad (3.2)$$

Proof. We discuss five possible cases:

Case 1: When $h > 2f-1$ and h is even.

Here we have

$$\zeta(T[h,f]) = \{e_1^{2h}, e_2^{6h}, \ldots, e_f^{6h}, e_{f+1}^{4h}\}.$$

Using formula (2.23), the NSC number of $T[h,f]$ is given by

$$\begin{aligned}\eta(T[h,f]) =&[(2h)(4h)+(2h)(4h)(2)+\dots+(2h)(6h)(f)]+[(4h)(4h)+\dots\\&+(4h)(6h)(f-1)]+\dots+[(4h)(6h)].\end{aligned}$$

After simplification, we get

$$\begin{aligned}\eta(T[h,f]) &= 18h^2f^2-10h^2f+6h^2f(f-1)(f-2)\\&=2h^2f[3f^2+1].\end{aligned}$$

Case 2: When $h>2f-1$ and h is odd.

In this case, we have

$$\zeta(T[h,f]) \quad = \quad \{e_1^{6h}, e_2^{6h}, \dots, e_f^{6h}\}.$$

Using (2.23), the NSC number of $T[h,f]$ is given by

$$\begin{aligned}\eta(T[h,f]) &= 18h^2f^2[(1)(2)+\dots+(f-2)(f-1)\\&+f(f-1)]\\&=6h^2f(f+1)(f-1).\end{aligned}$$

Case 3: When $h\in\{2f-2,2f-1\}$.

The eccentricity sequence of $T[h,f]$ in this case is given by

$$\zeta(T[h,f]) =\{e_1^{2h}, e_2^{4h}, e_3^{4h}, e_4^{2h}, e_5^{2h}, e_6^{6h}, \dots, e_{f+2}^{6h}, e_{f+3}^{4h}\}. \tag{3.3}$$

Using formula (2.23), the NSC number of $T[h,f]$ is given by

$$\begin{aligned}\eta(T[h,f]) =&2h[4h+4h\{2\}+2h\{3\}+2h\{4\}+6h\{5\}+6h\{6\}+\dots+6h\{f+1\}\\&+4h\{f+2\}]+4h[4h+2h\{2\}+2h\{3\}+6h\{4\}+6h\{5\}+\dots+6hf\\&+4h\{f+1\}]+4h[2h+2h\{2\}+6h\{3\}+6h\{4\}+\dots+6h\{f-1\}\\&+4h\{f\}]+2h[2h+6h\{2\}+6h\{3\}+\dots+6h\{f-2\}+4h\{f-1\}]\\&+2h[6h+6h\{2\}+6h\{3\}+\dots+6h\{f-3\}+4h\{f-2\}]+6h[6h+\\&+6h\{3\}+\dots+6h\{f-4\}+4h\{f-3\}]+6h[6h+6h\{2\}+6h\{3\}\\&+\dots+6h\{f-5\}+4h\{f-4\}]+\dots+6h[6h+4h\{2\}]+6h[4h].\end{aligned}$$

After simplification, we obtain:

$$\eta(T[h,f]) = h^2[6f^3 + 122f - 216]. \tag{3.4}$$

Case 4: When $h < 2f-2$ and f is even.

In this case, for $T[h,f]$ we have

$$\zeta(T[h,f]) = \{e_1^{2h}, e_2^{4h}, e_3^{4h}, e_4^{2h}, e_5^{2h}, \ldots, e_{2f-2}^{4h}, e_{2f-1}^{4h}, e_{2f}^{2h}\}.$$

Using formula (2.23), the NSC number of $T[h,f]$ is given by

$$\begin{aligned}\eta(T[h,f]) = \; & 4h^2\Bigg(\Bigg[\frac{(2f-1)(2f)}{2} + (1+2+5+6+\cdots+(2f-3)+(2f-2))\Bigg] \\ & +2\Bigg[\frac{(2f-2)(2f-1)}{2} + (1+4+5+\cdots+(2f-4)+(2f-3))\Bigg] \\ & +2\Bigg[\frac{(2f-3)(2f-2)}{2} + (3+4+7+8+\cdots+(2f-5)+(2f-4))\Bigg] \\ & +\Bigg[\frac{(2f-4)(2f-3)}{2} + (2+3+6+7+\cdots+(2f-6)+(2f-5))\Bigg] \\ & +\Bigg[\frac{(2f-5)(2f-4)}{2} + (1+2+5+6+\cdots+(2f-7)+(2f-6))\Bigg] \\ & +\cdots+\Bigg[\frac{3(3+1)}{2} + (1+2)\Bigg] + 2\Bigg[\frac{2(2+1)}{2} + (1)\Bigg] + 2\Bigg[\frac{1(1+1)}{2}\Bigg]\Bigg).\end{aligned}$$

After simplification we get

$$\eta(T[h,f]) = 4h^2\left[2f^3 + \frac{f}{2}(2f^2-5)\right]. \tag{3.5}$$

Case 5: When $h < 2f-2$ and f is odd.

In this case, the eccentricity sequence of $T[h,f]$ is given by

$$\zeta(T[h,f]) = \{e_1^{2h}, e_2^{4h}, e_3^{4h}, e_4^{2h}, e_5^{2h}, \ldots, e_{2f-2}^{2h}, e_{2f-1}^{2h}, e_{2f}^{4h}\}.$$

By formula (2.23), the NSC number of $T[h,f]$ is given by

$$
\begin{aligned}
\eta(T[h,f]) = {} & 2h[4h + 4h\{2\} + 2h\{3\} + 2h\{4\} + 4h\{5\} + 4h\{6\} + \cdots + 2h\{2f-3\} \\
& + 2h\{2f-2\} + 4h\{2f-1\}] + 4h[4h + 2h\{2\} + 2h\{3\} + 4h\{4\} + 4h\{5\} \\
& + \cdots + 2h\{2f-4\} + 2h\{2f-3\} + 4h\{2f-2\}] + 4h[2h + 2h\{2\} + 4h\{3\} \\
& + 4h\{4\} + \cdots + 2h\{2f-5\} + 2h\{2f-4\} + 4h\{2f-3\}] + 2h[2h \\
& + 4h\{2\} + 4h\{3\} + \cdots + 2h\{2f-6\} + 2h\{2f-5\} + 4h\{2f-4\}] + \ldots \\
& + 2h[2h + 4h\{2\} + 4h\{3\} + 2h\{4\} + 2h\{5\} + 4h\{6\}] + 2h[4h + 4h\{2\} \\
& + 2h\{3\} + 2h\{4\} + 4h\{5\}] + 4h[4h + 2h\{2\} + 2h\{3\} + 4h\{4\}] + 4h \\
& [2h + 2h\{2\} + 4h\{3\}] + 2h[2h + 4h\{2\}] + 2h[4h].
\end{aligned}
$$

Simplifying above, we obtain

$$\eta(T[h,f]) = 4h^2[3f^3 - f]. \tag{3.6}$$

This completes the proof. □

Remark. *For V-Phenylenic nanotori, the graph become self-centered. Therefore non-self-centrality number of V-phynelenic nanotori is zero.*

3.2 TUC_4C_8 nanotubes

In this section, we compute the non-self centrality number of TUC_4C_8 nanotubes. In the structure of TUC_4C_8 nanotube, every C_4 cycle is adjacent to four C_8 cycles. We will denote TUC_4C_8 nanotube by $H[u,v]$, where s is the number of octagones in a fixed row and t denotes the sum of C_4 and C_8 cycles in a fixed column (see Figure 3.3).

Consider

$$X = \{w \in \mathcal{V}(H[s,t]) \mid \deg(w) = 2\},$$

$$Y = \{w \in \mathcal{V}(H[s,t]) \mid \deg(w) = 3\}.$$

Then $|X| = 4s$ and $|Y| = 4st$. Also

$$|\mathcal{E}(H[s,t])| = 2s(3t+2).$$

Remark. *The graph $H[s,t]$ becomes self-centered for $t = 1$. Therefore the non-self-centrality number of $H[s,1]$ is zero.*

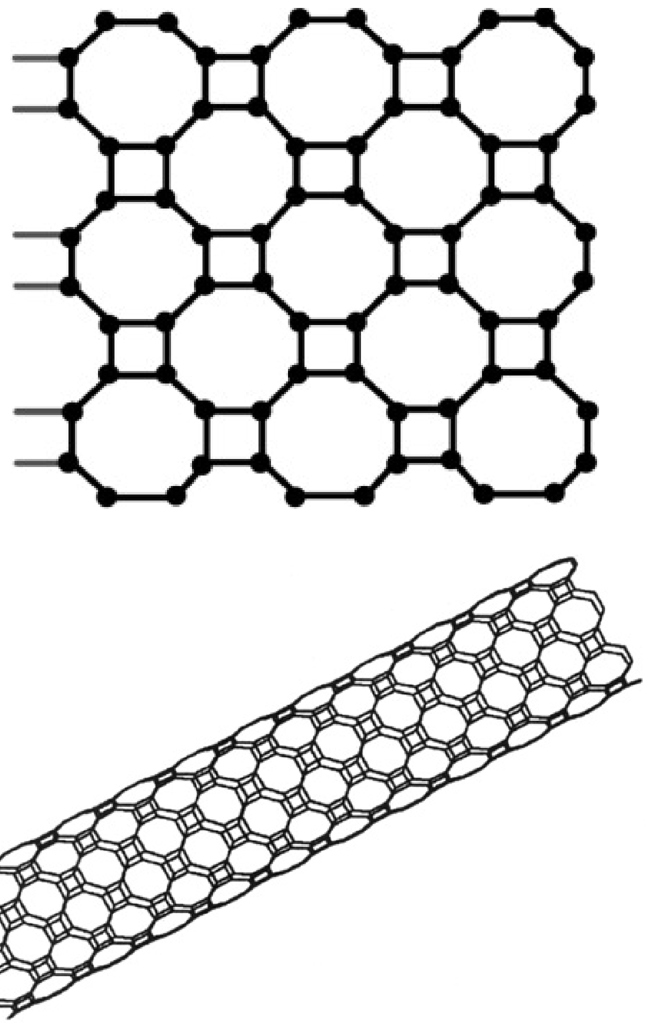


Figure 3.3: 2-D and 3-D structure of TUC_4C_8 Nanotube

Theorem 3.2.1. *Assume that $s \geq 2$ and t is an odd integer. Then the NSC number of TUC_4C_8 nanotube is given by*

$$\eta(H[s,t]) = \frac{8s^2t}{3}(t+1)(t+2). \tag{3.7}$$

Proof. The eccentricity sequence of $H[s,t]$ is given by

$$\zeta(H[s,t]) \quad = \quad \{e_1^{4s}, e_2^{4s}, \ldots, e_t^{4s}, e_{t+1}^{4s}\}. \tag{3.8}$$

Using formula (2.23) the NSC of $H[s,t]$ is given by

$$\begin{aligned}\eta(H[s,t]) &= 16s^2[1+2+3+\cdots+(t)]+16s^2[1+2+3+\cdots+(t-1)]+\ldots\\ &\quad +16s^2[1+2]+16u^2\\ &= 16s^2[1\cdot 2+2\cdot 3+\cdots+t(t-1)+(t+1)t]\\ &= \frac{8s^2t}{3}(t+1)(t+2).\end{aligned}$$

This completes the proof. □

Remark. *The graph of TUC_4C_8 nanotori, shown in Figure 3.4, is self-centered. Therefore non-self-centrality number of nanotori is zero.*

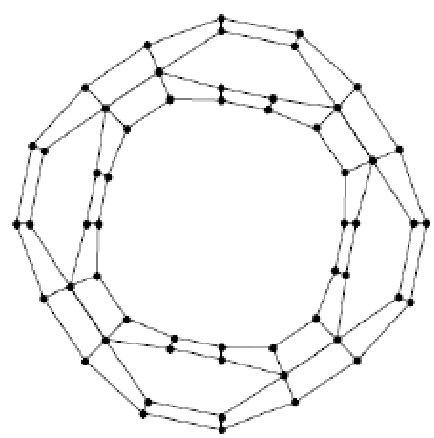


Figure 3.4: TUC_4C_8 nanotori

3.3 Conclusion

In this paper, we computed general formulas for the non-self-centrality number of V-Phenylenic and $TUC_4C_8(R)$ nanotubes. For future study, we can calculate the non-self-centrality number of other molecular structures such as α-Boron nanotubes, some layer structures and dendimers.

Chapter 4

Non-self-centrality number of fixed degree trees

Let $\mathcal{T}(n, \Delta)$, $\Delta \geq 4$ be the class of n-vertex trees with fixed maximum degree Δ. In this paper, we address the problem proposed by Xu et al. [9] and find a tree in $\mathcal{T}(n, \Delta)$ with largest NSC number.

4.1 Largest NSC number of trees with fixed degree

In this section, we determine a tree with largest NSC number in $\mathcal{T}(n, \Delta)$. A tree $T \in \mathcal{T}(n, \Delta)$ is a broom if Δ pendant vertices are adjacent to one end-vertex of a path with $n - \Delta$ vertices. Thus, if T is a broom then $d(T) = n - \Delta + 1$. An n-vertex broom with maximum degree Δ is denoted by $B_{n,\Delta}$. A broom $B_{10,4}$ is shown in Figure 4.1. The eccentricity sequence of $B_{n,\Delta}$ is given by

$$\zeta(T) \quad = \quad \{e_1^{\Delta}, e_2^2, \ldots, e_{k-1}^2, e_k^{l_k}\}. \tag{4.1}$$

Since center of $B_{n,\Delta}$ is K_1 or K_2, we have $l_k = 1$ if $d(B_{n,\Delta})$ is even and $l_k = 2$ if $d(B_{n,\Delta})$ is odd.

An n-vertex 1-broom B in $\mathcal{T}(n, \Delta)$ is a tree whose $\Delta - 1$ pendant vertices are adjacent to one end-vertex of a path with $n-\Delta$ vertices and has a unique pendant vertex with eccentricity less than $d(B)$. The eccentricity sequence of 1-broom $B \in \mathcal{T}(n, \Delta)$ is given by

$$\zeta(B) \quad = \quad \{e_1^{\Delta}, e_2^2, \ldots, e_{p-1}^2, e_p^3, e_{p+1}^2, \ldots, e_{k-1}^2, e_k^{l_k}\}, \tag{4.2}$$

where $2 \leq p \leq (k-1)$. Also $d(B) = n - \Delta$. The class of n-vertex 1-brooms with maximum degree Δ is denoted by $\tilde{\mathcal{B}}_n^{\Delta}$. A 1-broom $B \in \tilde{\mathcal{B}}_{10}^4$ is shown in Figure 4.2.

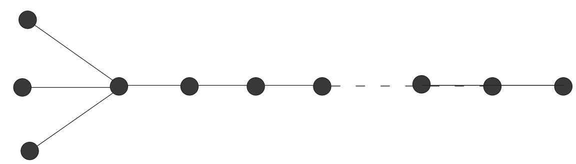


Figure 4.1: A broom $B_{10,4}$

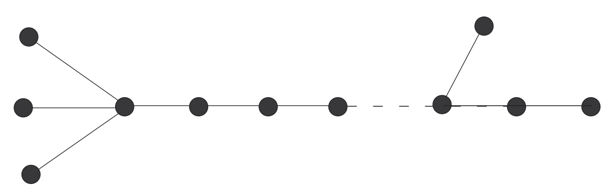


Figure 4.2: A 1-broom in $\tilde{\mathcal{B}}_{10}^4$

In the following Lemma, we calculate NSC number of the broom $B_{n,\Delta}$.

Lemma 4.1.1. *Let r be the radius of $B_{n,\Delta}$. Then NSC number of $B_{n,\Delta}$ is given by*

$$\eta(B_{n,\Delta}) = \begin{cases} r^2(\Delta) + r(r-1)\left(\dfrac{2r-1}{3}\right) & \text{if } d(B_{n,\Delta}) \text{ is even,} \\ \\ r(r-1)\left(\dfrac{3\Delta + 2(r-2)}{3}\right) & \text{if } d(B_{n,\Delta}) \text{ is odd.} \end{cases} \tag{4.3}$$

Proof. We consider two cases:

Case 1. When $d(B_{n,\Delta})$ is even.

In this case, the eccentricity sequence of $B_{n,\Delta}$ is given by

$$\zeta(B_{n,\Delta}) = \{e_1^{\Delta}, e_2^2, e_3^2, \ldots, e_{k-1}^2, e_k^1\}.$$

Using formula (2.23), we obtain

$$\begin{aligned}\eta(B_{n,\Delta}) &= 2\Delta[1+2+\cdots+(k-2)]+\Delta(k-1)+4[1+2+\cdots+(k\\&\quad-3)]+2(k-2)+\cdots+4[1+2]+2(3)+4[1]+2(2)+2(1)\\&= 2\Delta\left[\frac{(k-2)(k-1)}{2}\right]+\Delta(k-1)+\frac{2}{3}(k-3)(k-2)(k-1)+\\&\quad\frac{2(k-2)(k-1)}{2}.\end{aligned}$$

After simplification, we can write

$$\eta(B_{n,\Delta}) \;=\; \Delta(k-1)^2+(k-2)(k-1)\left(\frac{2k-3}{3}\right). \qquad (4.4)$$

Since $d(B_{n,\Delta})$ is even therefore $k=r+1$. Now equation (4.4) can be written as

$$\eta(B_{n,\Delta}) \;=\; \Delta r^2+r(r-1)\left(\frac{2r-1}{3}\right).$$

Case 2. When $d(B_{n,\Delta})$ is odd.

In this case, the eccentricity sequence of $B_{n,\Delta}$ is given by

$$\zeta(B_{n,\Delta})=\{e_1^{\Delta},e_2^2,e_3^2,\ldots,e_{k-1}^2,e_k^2\}.$$

Again using the formula (2.23), we obtain

$$\begin{aligned}\eta(B_{n,\Delta}) &= 2\Delta[1+2+\cdots+(k-1)]+4[1+2+\cdots+(k-2)]+\cdots+\\&\quad 4[1+2]+4[1]\\&= 2\Delta\left[\frac{k}{2}(k-1)\right]+\frac{2}{3}(k-2)k(k-1).\end{aligned}$$

After simplification, we obtain

$$\eta(B_{n,\Delta}) \;=\; \Delta k(k-1)+\frac{2}{3}(k-2)k(k-1). \qquad (4.5)$$

Since $d(B_{n,\Delta})$ is odd therefore $k=r$. Now we can write equation (4.5) as

$$\eta(B_{n,\Delta}) \;=\; r(r-1)\left(\frac{3\Delta+2(r-2)}{3}\right).$$

The proof is complete. □

In next lemma, we give NSC number a 1-broom in $\tilde{\mathcal{B}}_n^{\Delta}$.

Lemma 4.1.2. *Let $B \in \tilde{\mathcal{B}}_n^{\Delta}$ be a 1-broom with radius r and eccentricity sequence given by (4.2). Then NSC number of B is given by*

$$\eta(B) = \begin{cases} \frac{1}{3}r(r-1)(2r-1) + \Delta r^2 + (p-1)(p-2+\Delta) \\ +(r+1-p)^2 & \text{if } d(B) \text{ is even,} \\ \\ \Delta r(r-1) + (p-1)(p-2+\Delta) + \frac{2}{3}(r-1)r(r-2) \\ +(r-p)(r+1-p) & \text{if } d(B) \text{ is odd.} \end{cases} \tag{4.6}$$

Proof. Using formula (2.23), the NSC number of B is given by

$$\begin{aligned} \eta(B) &= l_1[l_2(1) + l_3(2) + \cdots + l_p(p-1) + \cdots + l_{k-1}(k-2) + l_k(k-1)] \\ &\quad + l_2[l_3(1) + l_4(2) + \cdots + l_p(p-2) + \cdots + l_{k-1}(k-3) + l_k(k-2)] \\ &\quad + \cdots + l_{p-1}[l_p(1) + l_{p+1}(2) + \cdots + l_{k-1}(k-p) + l_k(k-p+1)] + \\ &\quad l_p[l_{p+1}(1) + l_{p+2}(2) + \cdots + l_{k-1}(k-p-1) + l_k(k-p)] + l_{p+1}[l_{p+2} \\ &\quad (1) + \cdots + l_{k-1}(k-p-2) + l_k(k-p-1)] + \cdots + l_{k-3}[l_{k-2}(1) + \\ &\quad l_{k-1}(2) + l_k(3)] + l_{k-2}[l_{k-1}(1) + l_k(2)] + l_{k-1}l_k(1) \\ &= 2\Delta\left[\frac{(k-2)(k-1)}{2}\right] + \Delta(p-1) + \Delta l_k(k-1) + 4\Bigg[[1 + 2 + \cdots + \\ &\quad (k-3] + \cdots + [1 + 2 + \cdots + (k-p)] + [1 + 2 + \cdots + (k-p-1)] \\ &\quad + [1 + 2 + \cdots + (k-p-2)] + \cdots + [1+2] + [1]\Bigg] + 2l_k[(k-2) + \\ &\quad \cdots + 3 + 2 + 1] + 2[(p-2) + \cdots + 1] + l_k(k-p) + 2[1 + 2 + \cdots + \\ &\quad (k-p-1)] \\ &= \Delta(p-1) + \Delta(k-1)(k-2) + l_k\Delta(k-1) + \frac{2}{3}(k-1)(k-3)(k-2) \\ &\quad + l_k(k-1)(k-2) + (p-1)(p-2) + (k-1-p)(k-p) + l_k(k-p). \end{aligned}$$

If $d(B)$ is even then $l_k = 1$ and $k = r+1$. Thus, we obtain

$$\eta(B) = \frac{1}{3}(r-1)r(2r-1) + \Delta r^2 + (p-1)(p+\Delta-2) + (1+r-p)^2.$$

If $d(B)$ is odd then $l_k = 2$ and $k = r$. Thus, we obtain

$$\eta(B) = (p-1)(p+\Delta-2) + \Delta r(r-1) + \frac{2}{3}(r-1)r(r-2) + (r-p)(r+1-p).$$

This completes the proof. □

In next lemma, we prove that NSC number of broom $B_{n,\Delta}$ is greater than any 1-broom in $\tilde{\mathcal{B}}_n^\Delta$.

Lemma 4.1.3. *For $n \geq 4$, we have $\eta(B_{n,\Delta}) > \eta(B)$ for any $B \in \tilde{\mathcal{B}}_n^\Delta$.*

Proof. Consider an n-vertex 1-broom $B \in \tilde{\mathcal{B}}_n^\Delta$. We divide the proof into two cases:
Case 1. When $d(B)$ is odd.

In this case, the eccentricity sequence of B is of the form

$$\zeta(B) = \{e_1^\Delta, e_2^2, \ldots, e_{p-1}^2, e_p^3, e_{p+1}^2, \ldots, e_r^2\}. \tag{4.7}$$

We know that $d(B) = n - \Delta$ and $d(B_{n,\Delta}) = n - \Delta + 1$. Hence $d(B_{n,\Delta})$ is even with the eccentricity sequence

$$\zeta(B_{n,\Delta}) = \{(e_1+1)^\Delta, e_1^2, e_2^2, \ldots, e_r^1\}. \tag{4.8}$$

Now using equations (4.7) and (4.8) and formula (2.23), we have

$$\eta(B_{n,\Delta}) - \eta(B) = \Delta(r+1-p) + 2[(r+1-p)(p-1)].$$

It is easy to see that

$$\Delta(r+1-p) + 2[(p-1)(r+1-p)] > 0.$$

Therefore, $\eta(B_{n,\Delta}) > \eta(B)$.
Case 2. When $d(B)$ is even.

In this case the eccentricity sequence of B is given by

$$\zeta(B) = \{e_1^\Delta, e_2^2, \ldots, e_{p-1}^2, e_p^3, e_{p+1}^2, \ldots, e_r^1\} \tag{4.9}$$

and hence $d(B_{n,\Delta})$ is odd. Therefore, the eccentricity sequence of $B_{n,\Delta}$ is given by

$$\zeta(B_{n,\Delta}) = \{(e_1+1)^{\Delta}, (e_2+1)^2, \ldots, (e_r+1)^2\}. \tag{4.10}$$

Now using equations (4.9) and (4.10) we can easily prove that

$$\eta(B_{n,\Delta}) > \eta(B).$$

This finishes the proof. □

It is obvious to see that corresponding to any n-vertex tree T, there is an n-vertex caterpillar F satisfying $\zeta(T) = \zeta(F)$ and vice versa. For convenience, we will use caterpillars in proving results. In next lemmas, we will construct a tree $T_1 \in \mathcal{T}(n,\Delta)$ from a given tree $T \in \mathcal{T}(n,\Delta)$ such that $\eta(T) < \eta(T_1)$.

Lemma 4.1.4. *Let $T \in \mathcal{T}(n,\Delta)$ such that $T \ncong B_{n,\Delta}$, $T \notin \tilde{\mathcal{B}}_n^{\Delta}$ and*

$$\zeta(T) \;=\; \{e_1^{l_1}, e_2^{l_2}, \ldots, e_p^{l_p}, \ldots, e_k^{l_k}\}, \tag{4.11}$$

where $2 \le p \le (k-1)$ and $l_1, l_p > 2$. Then there exists $T_1 \in \mathcal{T}(n,\Delta)$ with $d(T_1) = d(T)+2$ and $\eta(T_1) > \eta(T)$.

Proof. Let F be an n-vertex caterpillar satisfying $\zeta(F) = \zeta(T)$. Also let P be a diametrical x,y-path in F and u, v be the neighbors of x, y on P, respectively. Now we consider following cases:

Case 1. When $l_1(T) \neq \Delta$.

Firstly, assume that $l_1(T) < \Delta$. Since $T \ncong B_{n,\Delta}$ and $T \notin \tilde{\mathcal{B}}_n^{\Delta}$, therefore there exist two pendant vertices w_1, w_2 in F other than x and y such that $e(w_1) = e_1$ and $e(w_2) = e_p$, where p is the least integer for which $l_1 + l_p \ge 6$. Let z_1 and z_2 be the neighbors of w_1 and w_2 on P, respectively. Also, let xua be a path of length 2 on P. Now construct a caterpillar F_1 as follows

$$F_1 \cong \{F - \{w_1z_1, w_2z_2\}\} \cup \{uw_1, w_1a, yw_2\}. \tag{4.12}$$

If $p = 2$ then the eccentricity sequence of F_1 is given by

$$\zeta(F_1) = \{(e_1+2)^{l_1-1}, (e_1+1)^2, (e_2+1)^{l_2-1}, \ldots, (e_k+1)^{l_k}\}. \tag{4.13}$$

From equation (4.13) it is clear that $d(F_1) = d(F) + 2$. Now by formula (2.23), the NSC number is given by

$$\eta(F_1) \quad = \quad \eta(F) + \sum_{i=2}^{k} l_1 l_i - 2. \tag{4.14}$$

Since $l_i \geq 2$ for all $1 \leq i \leq (k-1)$, it holds that

$$\sum_{i=2}^{k} l_1 l_i - 2 > 0.$$

Therefore, $\eta(F_1) > \eta(F)$. Now we will prove the result for $p \geq 3$. In this case, the eccentricity sequence of F_1 is given by

$$\begin{aligned}\zeta(F_1) \quad = \quad & \{(e_1+2)^{l_1-1}, (e_1+1)^2, (e_2+1)^2, \ldots, (e_{p-1}+1)^2, (e_p+1)^{l_p-1}, \\ & (e_{p+1}+1)^{l_{p+1}}, \ldots, (e_k+1)^{l_k}\}. \end{aligned} \tag{4.15}$$

From equation (4.15), it is seen that $d(F_1) = d(F) + 2$. Here we have following two possibilities:

(i) If $e_1 \neq e_p$ then $l_1 = 3$. Since p is the least integer for which $l_1 + l_p \geq 6$, we have $l_i = 2$, where $2 \leq i \leq (p-1)$. Therefore by using formula (2.23) and after simplification, we obtain

$$\eta(F_1) = \eta(F) + (p-2)(l_1-1) + \sum_{i=p}^{k} l_i(l_1 - 2 + p), \tag{4.16}$$

where

$$(p-2)(l_1-1) + \sum_{i=p}^{k} l_i(l_1 - 2 + p) > 0.$$

Therefore $\eta(F_1) > \eta(F)$.

(ii) If $e_1 = e_p$ then $l_1 > 3$. Hence the eccentricity sequence (4.15) reduces to

$$\zeta(F_1) = \{(e_1+2)^{l_1-2}, (e_1+1)^2, (e_2+1)^{l_2}, \ldots, (e_k+1)^{l_k}\}.$$

Therefore using formula (2.23), we obtain

$$\eta(F_1) = \eta(F) + 2(l_1-2) + \sum_{i=2}^{k} l_i(l_1-2), \tag{4.17}$$

where

$$2(l_1 - 2) + \sum_{i=2}^{k} l_i(l_1 - 2) > 0.$$

Hence $\eta(F_1) > \eta(F)$.

Next assume that $l_1(T) > \Delta$. We choose two pendant vertices w_1 and w_2 such that $e(w_1) = e_1$ and $e(w_2) = e_p$, where p is the least integer such that $l_1 + l_p > \Delta$. If $l_1 - \Delta > 1$ then $e_1 = e_p$; otherwise $e_1 \neq e_p$. The eccentricity sequence in this case is similar to the sequence given in (4.13). Hence $d(F_1) = d(F) + 2$ and $\eta(F_1) > \eta(F)$.

Case 2. When $l_1(T) = \Delta$.

If $2 < deg_F(u), deg_F(v) < \Delta$ then remove all pendant vertices adjacent to v, except y, and attach them to u such that $deg_F(v) = 2$ and $deg_F(u) = \Delta$. Otherwise, choose u, v such that $deg_F(u) = \Delta$ and $deg_F(v) = 2$ and proceed as follows.

We choose y_1 and y_2 such that $e(y_1) = e_p$ and $e(y_2) = e_q$, where p and q are the least integers for which $l_p + l_q \geq 6$ and $p, q \geq 2$. Then by applying transformation (4.12), to obtain a caterpillar F_1 with eccentricity sequence given by

$$\zeta(F_1) = \{(e_1 + 2)^{l_1}, (e_1 + 1)^2, (e_2 + 1)^2, \ldots, (e_{p-1} + 1)^2, (e_p + 1)^{l_p - 1}, (e_{p+1} + 1)^2, \ldots, (e_{q-1} + 1)^2, (e_q + 1)^{l_q - 1}, \ldots, (e_k + 1)^{l_k}\}. \quad (4.18)$$

Clearly $d(F_1) = d(F) + 2$. Here we have two possibilities:

(i) If $e_p \neq e_q$ then $l_p = 3$. Since p, q are the least integers for which $l_p + l_q \geq 6$, we have $l_i = 2$ for $i \in \{2, \ldots, (q-1)\} \setminus p$. Therefore, by formula (2.23) the NSC number of F_1 is given by

$$\eta(F_1) = \eta(F) + \Delta + \sum_{i=q+1}^{k} l_i[l_1 - 2 + q + p] + (\Delta - 2)(l_q + p) + \Delta q(l_q - 2) + 2[p(q-p) - 1] + l_q(q + p), \quad (4.19)$$

where

$$\Delta + \sum_{i=q+1}^{k} l_i[l_1 - 2 + q + p] + (\Delta - 2)(l_q + p) + \Delta q(l_q - 2) + 2[p(q-p) - 1] + l_q(q + p) > 0.$$

Hence $\eta(F_1) > \eta(F)$.

(ii) If $e_p = e_q$ then $l_p > 3$. Hence the eccentricity sequence in equation (4.18) reduces to

$$\zeta(F_1) = \{(e_1+2)^{l_1}, (e_1+1)^2, (e_2+1)^{l_2}, \ldots, (e_p+1)^{l_p-2}, \ldots, (e_k+1)^{l_k}\}. \tag{4.20}$$

Therefore, by formula (2.23) and using the fact that $l_i = 2$ for each $2 \le i \le (p-1)$, we have

$$\eta(F_1) = \eta(F) + l_1(l_p-2) + 2(p-1)(l_p-2) + \sum_{i=p+1}^{k} l_i(l_1+2p-2), \tag{4.21}$$

where

$$l_1(l_p-2) + 2(p-1)(l_p-2) + \sum_{i=p+1}^{k} l_i(l_1+2p-2) > 0.$$

Hence $\eta(F_1) > \eta(F)$.

Let $T_1 \in \mathcal{T}(n,\Delta)$ be a tree corresponding to the caterpillar F_1 with $\zeta(T_1) = \zeta(F_1)$. Thus

$$N(T_1) > N(T).$$

This finishes the proof. □

Lemma 4.1.5. *Let $T \in \mathcal{T}(n,\Delta)$ such that $T \ncong B_{n,\Delta}$, $T \notin \tilde{\mathcal{B}}_n^{\Delta}$ and*

$$\zeta(T) \;=\; \{e_1^2, e_2^2, \ldots, e_{p-1}^2, e_p^{l_p}, e_{p+1}^2, \ldots, e_{q-1}^2, e_q^{l_q}, \ldots, e_k^{l_k}\}, \tag{4.22}$$

where $2 \le p \le q \le (k-1)$ and $l_p, l_q > 2$. Then there exists $T_1 \in \mathcal{T}(n,\Delta)$ with $\eta(T_1) > \eta(T)$. Moreover

(a) *If $3 < l_p < \Delta$ then $d(T_1) = d(T) + 2$*

(b) *If $l_p \ge \Delta$ then $l_1(T_1) = \Delta$*

(c) *If $l_p = 3$ and $3 \le l_q < \Delta$ then $d(T_1) = d(T) + 2$*

(d) *If $l_p = 3$ and $l_q \ge \Delta$ then $l_1(T_1) = \Delta$.*

Proof. Let F be a caterpillar such that $\zeta(F) = \zeta(T)$. Also let P be a diametrical x, y-path in F and u be the neighbor of x on P and xuw be a path of length 2 on P. Here we discuss two different cases:

(a) When $3 < l_p < \Delta$.

Here we choose two pendant vertices w_1, w_2 other than x and y. Also let z_1 and z_2 be the neighbors of w_1, w_2 on P, respectively. Now by applying the transformation in Lemma 4.1.4 (a) to obtain a caterpillar F_1 with

$$\begin{aligned}\zeta(F_1) = \{&(e_1+2)^2, (e_1+1)^2, (e_2+1)^2, \ldots, (e_{p-1}+1)^2, (e_p+1)^{l_p-2}, \\ &\ldots, (e_k+1)^{l_k}\}.\end{aligned} \tag{4.23}$$

From the above equation we can see that $d(F_1) = d(F) + 2$. Now using formula (2.23), we have

$$\eta(F_1) = \eta(F) + 2p \sum_{i=p+1}^{k} l_i + 2p(l_p - 2), \tag{4.24}$$

where

$$2p \sum_{i=p+1}^{k} l_i + 2p(l_p - 2) > 0.$$

This implies $\eta(F_1) > \eta(F)$.

(b) When $l_p \geq \Delta$.

Let w_i be the pendant vertices in F other than x and y, where $1 \leq i \leq (\Delta - 2)$ and z' be the unique neighbor of w_i on P such that $e(w_i) = e_p$. Now construct a caterpillar F_1 such that

$$F_1 \cong \{F - \{w_1z', w_2z', \ldots, w_{\Delta-2}z'\}\} \cup \{w_1u, w_2u, \ldots, w_{\Delta-2}u\}. \tag{4.25}$$

Hence, the eccentricity sequence of F_1 is given by

$$\zeta(F_1) = \{e_1^{\Delta}, e_2^2, \ldots, e_{p-1}^2, e_p^{l_p-(\Delta-2)}, \ldots, e_k^{l_k}\}. \tag{4.26}$$

From equation (4.26), we have $l_1(F_1) = \Delta$. Now using formula (2.23), the NSC number is given by

$$\begin{aligned}\eta(F_1) &= \eta(F) + \sum_{i=p+1}^{k} l_i(\Delta-2)(i-i+p-1) + (p-1)(\Delta-2)(l_p - \\ &\quad (\Delta-2)-p) + 2(\Delta-2)\Big[1+2+\cdots+(p-2)\Big] \\ &= \eta(F) + (\Delta-2)(p-1)\Big[\sum_{i=p+1}^{k} l_i + (l_p-\Delta)\Big],\end{aligned}$$

where

$$(\Delta-2)(p-1)\Big[\sum_{i=p+1}^{k} l_i + (l_p-\Delta)\Big] > 0.$$

Therefore

$$\eta(F_1) > \eta(F).$$

(c) When $l_p = 3$ and $3 \leq l_q < \Delta$.

Since $l_p = 3$ and $l_q \geq 3$ therefore, there exist two pendant vertices w_1, w_2 in F other than x and y such that $e(w_1) = e_p$ and $e(w_2) = e_q$, where p and q are the least integers for which $l_p + l_q \geq 6$. Let z_1 and z_2 be the neighbors of w_1 and w_2 on P, respectively. Also, let xua be a path of length 2 on P. Now we can apply transformation in (4.12) to get a caterpillar F_1 having the eccentricity sequence

$$\begin{aligned}\zeta(F_1) = \{&(e_1+2)^2, (e_1+1)^2, (e_2+1)^2, \ldots, (e_{p-1}+1)^2, (e_p+1)^{l_p-1}, \\ &(e_{q+1}+1)^2, \ldots, (e_{q-1}+1)^{l_{q-1}}, (e_q+1)^{l_q-1}, (e_k+1)^{l_k}\}.\end{aligned} \tag{4.27}$$

From the above equation, we have $d(F_1) = d(F) + 2$. Using formula (2.23), we can easily see that $\eta(F_1) > \eta(F)$.

(d) When $l_q = 3$ and $l_q \geq \Delta$.

We choose vertices w_i, $1 \leq i \leq (\Delta-2)$ such that $e(w_1) = e_p$ and $e(w_i) = e_q$ for $2 \leq i \leq (\Delta-2)$, where q and p are the least integers for which $l_p + l_q \geq \Delta$. Now construct F_1 by applying the transformation (4.25). The eccentricity sequence of F_1 is given by

$$\zeta(F_1) = \{e_1^{\Delta}, e_2^2, \ldots, e_{p-1}^2, e_p^{l_p-1}, e_{p+1}^2, \ldots, e_{q-1}^2, e_q^{l_q-(\Delta-3)}, \ldots, e_k^{l_k}\}.$$

This implies $l_1(F_1) = \Delta$ and $d(F_1) = d(F)$. Hence by using formula (2.23), we can easily prove that $N(F_1) > N(F)$.

Let $T_1 \in \mathcal{T}(n, \Delta)$ be a tree corresponding to the caterpillar F_1. Then in $(a) - (d)$, we can write

$$\eta(T_1) > \eta(T).$$

This finishes the proof. □

Now we give our main result. We show that the broom $B_{n,\Delta}$ has largest NSC number among trees in $\mathcal{T}(n, \Delta)$.

Theorem 4.1.1. *Among all trees in $\mathcal{T}(n, \Delta)$, $n \geq 4$, the broom $B_{n,\Delta}$ has largest NSC number.*

Proof. Let $T \in \mathcal{T}(n, \Delta)$ with eccentricity sequence given by

$$\zeta(T) = \{e_1^{l_1}, e_2^{l_k}, \ldots, e_k^{l_k}\}.$$

We divide the proof into two cases:

Case 1. When $l_1(T) = 2$

Let s be the smallest integer with $l_s \geq \Delta$.

(a) If $l_p(T) = 2$ for each $i < s$ then by Lemma 4.1.5 (b), there exists $T_1 \in \mathcal{T}(n, \Delta)$ satisfying $l_1(T_1) = \Delta$ and $\eta(T_1) > \eta(T)$.

(b) If $l_p(T) \neq 2$ for some $p < s$ then by the choice of s, we have $3 \leq l_p < \Delta$. By Lemma 4.1.5 (a), there exists $T_1 \in \mathcal{T}(n, \Delta)$ such that $d(T_1) = d(T) + 2$ and $\eta(T_1) > \eta(T)$.

Case 2. When $l_1(T) \neq 2$

(a) If $l_1(T) = \Delta$ then by Lemma 4.1.4 (b), there exists $T_1 \in \mathcal{T}(n, \Delta)$ such that $d(T_1) = d(T) + 2$ and $\eta(T_1) > \eta(T)$.

(b) If $l_1(T) \neq \Delta$ then by Lemma 4.1.4 (a), there exists $T_1 \in \mathcal{T}(n, \Delta)$ such that $l_1(T_1) = 2$ or $l_1(T_1) = \Delta$ and $\eta(T_1) > \eta(T)$.

Now in Case 1 (a), if $T_1 \cong B_{n,\Delta}$ then we are done. If $T_1 \in \tilde{\mathcal{B}}_n^{\Delta}$ then by Lemma 4.1.3, we obtain required result. Otherwise, we apply Lemma 4.1.4 (b) on T_1 to get a tree $T_2 \in \mathcal{T}(n, \Delta)$ satisfying $d(T_2) = d(T_1) + 2$ and $\eta(T_2) > \eta(T_1)$.

In Case 1 (b), if $l_p(T_1) \neq 2$ for some $p < s$, we apply Lemma 4.1.5 (a) again on T_1 to get $T_2 \in \mathcal{T}(n, \Delta)$ satisfying $d(T_2) = d(T_1) + 2$ and $\eta(T_2) > \eta(T_1)$. If $l_p(T_1) = 2$ for each $p < s$, we apply Case 1 (a) to get $T_2 \in \mathcal{T}(n, \Delta)$ satisfying $l_1(T_2) = \Delta$ and $\eta(T_2) > \eta(T_1)$.

In Case 2 (a), if $T_1 \cong B_{n,\Delta}$ then we are done. If $T_1 \in \tilde{\mathcal{B}}_n^{\Delta}$ then by Lemma 4.1.3, we obtain required result. Otherwise, we apply Lemma 4.1.4 (b) on T_1 to get a tree $T_2 \in \mathcal{T}(n, \Delta)$ satisfying $d(T_2) = d(T_1) + 2$ and $\eta(T_2) > \eta(T_1)$.

In Case 2 (b), if $l_1(T_1) = 2$ we proceed like Case 1 to obtain a tree $T_2 \in \mathcal{T}(n, \Delta)$ satisfying $\eta(T_2) > \eta(T_1)$. If $l_1(T_1) = \Delta$, $T_1 \ncong B_{n,\Delta}$ and $T_1 \notin \tilde{\mathcal{B}}_n^{\Delta}$, we apply Lemma 4.1.4 (b) on T_1 to get a tree $T_2 \in \mathcal{T}(n, \Delta)$ satisfying $d(T_2) = d(T_1) + 2$ and $\eta(T_2) > \eta(T_1)$. Moreover, if $l_1(T_1) = \Delta$ and $T_1 \cong B_{n,\Delta}$ or $T_1 \in \tilde{\mathcal{B}}_n^{\Delta}$ then we obtain required result.

In this way, we obtain a finite sequence of trees $T_i \in \mathcal{T}(n, \Delta)$, $i = 1, 2, \dots, m$, satisfying

$$\eta(T) < \eta(T_1) < \eta(T_2) < \cdots < \eta(T_m),$$

such that $T_m \cong B_{n,\Delta}$ or $T_m \in \tilde{\mathcal{B}}_n^{\Delta}$. If $T_m \cong B_{n,\Delta}$ then we obtain the required result. If $T_m \in \tilde{\mathcal{B}}_n^{\Delta}$, then by Lemma 4.1.3, $\eta(T) < \eta(T_m) < \eta(B_{n,\Delta})$.
This finishes the proof. □

4.2 Conclusions

In this paper, we showed that the broom $B_{n,\Delta}$ has the largest NSC number in the class $\mathcal{T}(n, \Delta)$ and computed general formula for the NSC number of $B_{n,\Delta}$. For further research, one can find the extremal graphs with respect to NSC number in different classes of graphs such as class of trees with fixed pendant vertices and class of unicyclic graphs with fixed girth. Furthermore, trees with smallest NSC number in the class $\mathcal{T}(n, \Delta)$ can also be determined.

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