Some degree-distance based topological indices of nanotubes

by

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A thesis submitted to the

School of Natural Sciences (SNS),
National University of Sciences and Technology,
H-12, Islamabad, Pakistan

for the Degree of Master of Philosophy

January 2019

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A thesis
Submitted for the Degree of Master of Philosophy
in
Mathematics

Supervised by
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FORM TH-4

National University of Sciences & Technology

MS THESIS WORK

We hereby recommend that the dissertation prepared under our supervision by: Ramsha Javed, Regn No. 00000172986 Titled: Some degree-distance based topological indices of nanotubes accepted in partial fulfillment of the requirements for the award of **MS** degree.

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Dedicated

to my

Parents

Acknowledgments

In the Name of Allah, The Most Beneficent, The Merciful. All the praise to His Prophet Muhammad (Peace be upon him), who gave us vision, wisdom and courage to complete this thesis.

I would like to take this opportunity to pay my sincere gratitude to all those, without whom this thesis could have never been come to an existence. I want to express my humble regards to my advisor Dr. Rashid Farooq, for encouraging me to exert on the ideas I came across. His benevolent gesture has been a true comfort, throughout the span. I also recognize my G.E.C. named, Dr. Matloob Anwar and Dr. Muhammad Ishaq, for putting their effort to evaluate my thesis. I would like to express my deepest recognition to my parents for their ultimate support and countless prayers. I would like to thank my brother for being always there for me and to spread colors in my life. I would also like to extend my thanks to all the research scholars, and official staff of School of Natural Sciences, for their cooperation in various aspects. Above all, Im deeply indebted to the Almighty Allah, Who has made all things possible and showered His countless blessings on me.

I would like to pay my gratitude to my teachers, friends, colleagues and to my family. My humble regards to my mentor and advisor Dr. Rashid Farooq for always encouraging me during my stay, at School of Natural Sciences (SNS), National University of Sciences and Technology. Apart from helping in my research, he has also taught me to be honest and punctual in my daily life. He has also inspired me in becoming a true professional. I am also thankful to my Guidance and Examination Committee (GEC) members, Dr.

Matloob Anwar and Dr. Muhammad Ishaq.

I am also thankful to Mehar Ali Malik, my senior and mentor who helped me a-lot in my research. I wish him best of luck. I want to acknowledge my friends at NUST-SNS especially Shawana Maryum, Talmeez-ur-Rehman, Aqsa Maryum and Amna Sadiq making my time enjoyable.

Ramsha Javed

Abstract

The number of unordered pairs of vertices lying at distance 3 in a graph is known as its Wiener polarity index. It has demonstrated quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons and it is also related to the cluster coefficient of networks. In this thesis, we consider three variants of the graph of titanium dioxide TiO_2; TiO_2 nanotubes, their 2-dimensional lattices and nanotorus. For these graph families, we compute the number of pairs of vertices lying at distance one, two and three. We also calculate the values of m_u, m_v, n_u and n_v Using these computations, we compute the Wiener polarity and leap Zagreb indices of these graphs.We also compute several Szeged-type indices such as vertex-Szeged, edge-Szeged, edge-vertex Szeged, total Szeged, Padmaker-Ivan, revised Szeged and revised-edge Szeged indices of 2-dimensional lattices of titanium dioxide nanotubes. We also correct several results from the literature about Szeged type indices of these nanotubes.

Preface

Leonhard Euler (1707-1783) is considered to be the most prolific mathematician in history. Euler revealed his aptitude in mathematics while attending the University of Basel. By 1726, the 19-year-old Euler had finished his work at Basel and published his first paper in mathematics. Euler worked, wrote, and published at a furious rate throughout his lifetime. So it is no surprise that when Euler decided to analyze the problem of the Königsberg bridges, he not only found the answer, but also initiated the study of a brand new field in mathematics. A seemingly trivial problem that lead to an entire branch of mathematics is not unusual. Whereas, some areas of mathematics were developed to answer obviously important questions (for instance, calculus was developed by Isaac Newton (1642-1727) to help answer questions in physics and astronomy), others branches of mathematics had their origins in much less noble causes (the origination of probability is traced to letters exchanged by Pierre de Fermat (1601-1665) and Blaise Pascal (1623-1662) in which they discussed questions in gambling). Although the branch of mathematics known today as graph theory had its origins in a simpleminded puzzle that entertained the people of Königsberg, its eventual usefulness to mathematics has completely overshadowed its humble beginnings. For instance, chemists use graphical notation to represent chemical compounds; and physicists and engineers use graphical notation to represent electrical circuits. Graph theory is used in complex computer programs that control telephone switching systems. Graph theory is a part of a larger field of mathematics called topology. Topology is the study of the properties of geometric figures that are invariant (do not change) when undergoing transformations such as stretching or compression. Imagine drawing a geometric figure, such as a square or a circle, on a sheet of flexible material like rubber, and then stretching or compressing the rubber sheet. The properties of the square and circle that do not change during this stretching or compression fall under the study of topology. For this reason, topology is sometimes referred to as "rubber-sheet geometry."

During the past two decades, there has been a considerable progress in the applications of algebraic graph theory in chemistry. Graph theory is concerned with manipulations of structures and structural informations. This involves classification of structures, that is, their grouping into smaller lots, characterization of structures, which can be accomplished by enumeration of selected structural invariants, and ordering of structure, which implies a decision of which among two or more structures should be taken first in the sequence. The first two chapters of this thesis are devoted to some basic definitions and terminologies of graphs. In the first chapter, we discus the origins of Graph Theory. We also give the basic definitions of graph theory.

In the second chapter we give a brief history of chemical graph theory and some well-known topological indices mainly distance, degree and counting based topological indices. In the class of distance based topological indices, we give a brief introduction of Wiener index, Wiener polarity index and Szeged index. In the class of degree based of topological indices, we discuss Zagreb indices. In the counting related polynomials and topological indices, we give a brief introduction of counting polynomials and counting related index called the Padmakar-Ivan (PI) index.

In the third chapter, we give a brief introduction on the properties of titania nano-tubes, 2-D lattice and nanotori. We further show the calculations for Wiener Polarity index of titania nano-tubes, 2-D lattice and nanotori.

In the fourth chapter, we initially discuss the cuts required to assist in the solution of Szeged-type-Indices of titania 2-D lattice. The chapter comprises of detailed calculations required to find the Szeged-type indices such as, edge-Szeged index, vertex-Szeged index, edge-vertex-Szeged index, Total-Szeged index, and Padmaker-Ivan index.

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Chapter 1

Fundamentals of graph theory

This chapter discusses some of the basic concepts of graph theory. Some examples are given for the familiarity of the reader.

1.1 History of graph theory

Most of branches of mathematics come from basic problems of calculations and measurements, the ancestry of graph theory comes from mere puzzle like problems [53]. These problems caught the attention of mathematicians, as a result of which graph theory came into being. This subject has developed rapidly over the years. It has given many theoretical results of large variety, ranging from chemical structures to many economic problems.

The Königsberg bridges problem is considered as one of the first problems of graph theory. This problem has provided various basic concepts of the subject [53]. The first paper written on this subject was by Leonhard Euler in 1736 with its focus on the Königsberg bridge problem [16]. The Königsberg city was separated by a river into four land regions. There were seven bridges in the city joining different land regions. People of the area were not sure whether it was possible to figure out a way in which every bridge could be crossed only once in a single tour. It is not known who brought this problem to Euler's attention initially, as he had not visited the city of Königsberg. Historians have found that in one of the letters written by Carl Leonhard Gottlieb Ehler to Leonhard Euler, it was Ehler who asked Euler to produce a solution to the problem. After which Euler studied the problem by eliminating the nonessential parts of the map as shown in the Figure 1.1.

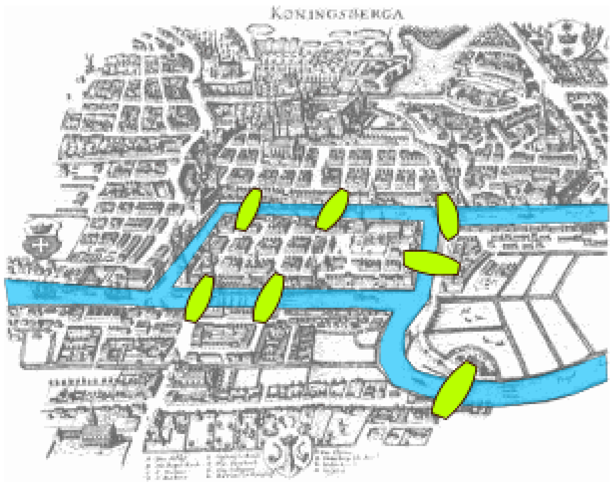

Figure 1.1: Königsberg bridge problem

In this process he exhausted all possibilities of existence of such path and also gave reasons as to why it was so. It is noteworthy that Euler did not produce the type of graphs we have today. It was one century later that such graphs made an appearance. This kind of a solution in which a real life problem was converted into a mathematical phenomenon opened the gates to the solution of many other practical problems. Graph theory has solved many such problems by converting the elements of certain problems into an abstract graphs containing vertices, edges and preserving the relationship between vertices.

1.2 Basic Definitions

Some basic definitions and terminologies regarding graph theory are given in this section. We start with the definition of a graph.

A graph, usually represented by the letter G, is a set that comprises of a pair of sets namely $V(G)$ (or simply V) and $E(G)$ (or simply E). A graph G with vertex set V and edge set E can also be denoted by $G = (V, E)$. The set V represents the set of vertices which is a collection of points. These points represent a variety of things depending upon the requirement of the graph. For example the vertices may represent atoms in a molecules, cities or people, depending upon the need of the problem. The set E represents the set of edges which is a collection of lines or relationships between the vertices. These lines may be curved or straight and may represent different things, such as bonds between atoms, roads between cities or relationships between people, etc. An edge e between the vertices u and v is commonly represented by uv. The vertices u and v in graph G are said to be adjacent, if they are joined by some edge. The line segment joining the vertices u and v represents the edge, denoted by uv, between them. The vertices u and v are the end-vertices of that edge. An edge e is said to be incident on v, only if v is an end-vertex of the edge e. The edge uv can also be denoted by the two-element subset $\{u, v\}$ of V, hence uv and vu denotes the same edge.

The number of edges incident on a vertex v in G represents its degree in the graph, denoted by $d_G(u)$. The edges that have a common end-vertex are called adjacent edges. The edges with no mutual end-points are called distinct or independent edges. Two edges with same end-vertices are called multiple edges. The edges that join a vertex with itself are called loops or self-loops. Graphs containing multiple edges or loops are called multigraphs. The graphs that neither contains multiple edges or loops are called simple graphs. A graph that has only one vertex is called a trivial graph. A graph that has no vertices is called a null graph. The total number of vertices in a graph G is termed as the order of graph and represented as $|V(G)| = n$. The total number of edges in $G = (V(G), E(G)$ is called the size of graph and is denoted by $|E(G)| = m$. A vertex with no adjacent vertices is called an isolated vertex and a vertex with only one adjacent vertex is called a leaf.

Example 1.1. Let us consider three students and two teachers such that each teacher must be assigned at-least one student. We label the students as a, b, c and teachers as x, y. If student a and c are assigned to teacher x and student b is assigned to the teacher y, then it is easier and convenient to represent the problem in the form of a graph, where $\{a, b, c, x, y\}$ is the set of vertices and the set $\{ax, cx, by\}$ is the set of edges which represent the allocation of the students to teachers. The order and size of the graph is 5 and 3, respectively.

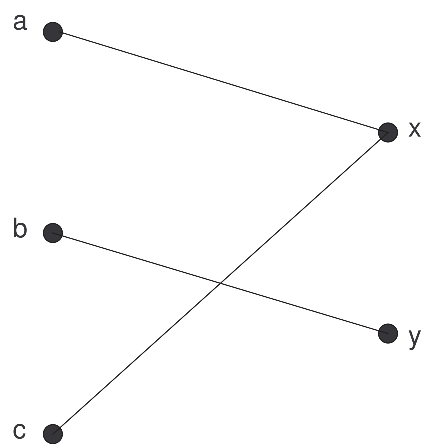

Figure 1.2: The graph of allocation of students to teachers.

A sequence of vertices $v_1, v_2, \ldots, v_n$ such that the consecutive vertices are adjacent represents a walk. The first vertex of the sequence is called initial vertex, whereas the last vertex is termed as the terminal vertex. A walk with all distinct edges is called a trail. If the vertices of walk are distinct, then it becomes a path. A walk whose initial and terminal vertices are same and all the other vertices are distinct is called a cycle. The order of a path or cycles is the number of vertices in it. The length of a path or cycle is determined by its number of edges. A subgraph H of a graph G is a graph with $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$.

The length of a shortest path between two vertices $u, v \in V$ in a graph G is called distance between u and v represented by $d_G(u, v)$. The eccentricity, $e_G(v)$ of a vertex v is defined as the maximum graph distance between a vertex v and all vertices $u \in G$ in the graph $u, v \in V$, such that $e_G(v) = \max_{u \in V} d_G(u, v)$. The maximum of all the vertex eccentricities in a graph G is called the diameter of G, denoted as $diam(G)$. A graph is said to be a connected graph if for every pair of vertices we can always find a path that connects them. If there exist vertices $u, v \in V$ such that there exists no path between them, then G is called a disconnected graph. A component is a subgraph C of graph G that is maximal connected subgraph of G, that is, there is no larger connected subgraph of G having C as a subgraph. Disconnected graphs contain more than one components. In a disconnected graph, the vertices have infinite eccentricity.

The neighbourhood of a vertex v in a graph G is denoted by $N_G(v)$ and defined as the set of all vertices of G which are adjacent to v. A non-negative number which indicates the number of graph edges in a graph G which are incident on a vertex $v \in V$ is called degree of v, denoted by $d_G(v)$. Mathematically, we can write $d_G(v) = |N_G(V)|$. The k-th neighborhood $N_G(v \mid k)$ of a vertex v in G is the set of vertices lying at distance k from v, that is, $N_G(v \mid k) = \{w \in V(G) \mid d_G(v, w) = k\}$. The k-th degree $d_G(v \mid k)$ of a vertex v in G is the cardinality $|N_G(v \mid k)|$. Note that for any $v \in V(G)$, there can be at most $n - 2$ (respectively, $n - 3$) vertices lying at distance 2 (respectively, 3) from v. Thus $d_G(v \mid 2) \leq n - 2$ and $d_G(v \mid 3) \leq n - 3$. The maximum degree of a graph G is the highest vertex degree in that graph, denoted as $\Delta(G)$, while the minimum degree is the smallest vertex degree in the graph, denoted as $\delta(G)$. A graph G is called regular or k-regular if it has the same highest and minimum degree, that is, $\Delta(G) = \delta(G) = k$. In this case, all vertices of G have degree k.

Example 1.2. Consider the graph shown in Figure 1.3. There exists no multiple edges or loops, hence it is a simple connected graph. In Figure 1.4, the edge set is given by $\{i, j, k, l, m, o, p, q\}$ and the vertex set is given by $\{a, b, c, d, e, f\}$. The edge i is a loop as it is connecting the vertex a with itself a, b, c, d and b, e, f are cycles of length 4 and 3, respectively. The edges p and q have the same end-vertices e and f, hence they form multiple edges.

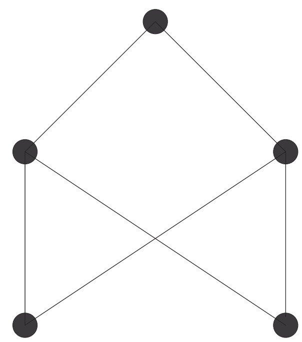

Figure 1.3: A simple graph.

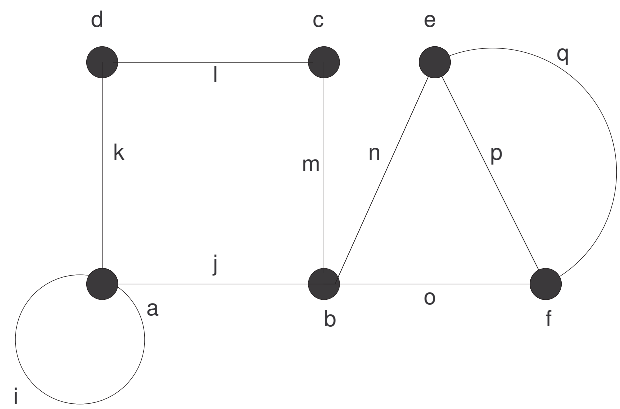

Figure 1.4: Graph representation of some basic definitions.

1.3 Basic operations

In this section we shall discuss some basic operations on graphs. These operations are used to construct new graphs with certain properties.

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. When a vertex is added to G such that $u \notin V(G)$ then the result produces a new graph G' such that $V(G') = V(G) \cup \{u\}$ is the new vertex set. The edge set remains unchanged. This process is called vertex addition or disjoint union of a graph and a vertex. Similarly, when a vertex v is deleted from a graph G, then the vertex v along with its incident edges are deleted forming the new graph, say H. The vertex and edge set of the new graph H are given by $V(H) = V(G) \setminus \{v\}$ and $E(H) = E(G) \setminus \{vw \in E(G) \mid w \in V(G)\}$. This process is called vertex deletion from a graph. For some $ab \notin E(G)$ and $a, b \in V(G)$, when ab is introduced as a new edge in G it formulates a new graph H' with edge set $E(H') = E(G) \cup \{ab\}$ and has no effect on the vertex set. This process is called edge addition. The deletion of an edge ab from G involves removal of the edge $ab \in E(G)$ such that the edge set of the new graph is given by $E(G) \setminus \{ab\}$ and has no effect on the vertex set.

A cut-vertex is a vertex such that its removal increases the number of components of the graph. A cut-edge is an edge such that its removal increases the number of components of the graph.

The smallest possible set of edges required to keep the graph connected is called the minimal edge set. There may exist more than one minimal edge sets.

Example 1.3. Consider the graph shown in Figure 1.5. The graph on the left consists of $V = \{a, b, c, d, e\}$ and $E = \{i, j, k, l, m\}$. After deletion of the bold edge l, the new graph has vertex set $\{a, b, c, d, e\}$ with edge set $\{i, j, k, m\}$. When the vertex c is deleted from the graph, the new graph has vertex set $\{a, b, d, e\}$ and edge set $\{i, j, m\}$.

1.4 Graph isomorphism

A graph may exists in various shapes and structures. Such graphs that retain the same set of vertices and edges but vary in shape are said to be isomorphic to each other. These graphs fulfill some conditions. Consider two simple graphs, namely G and H. There exists a vertex bijection $f : V_G \rightarrow V_H$ such that the bijection preserves adjacency and non-adjacency. Then for every pair of vertices in G, then of u and v are adjacent in G then $f(u)$ and $f(v)$ are adjacent in H. For the isomorphism between these graphs, there must exist bijection function.

In other words, both graphs must have same number of vertices, edges, components, loops and parallel edges, etc. Along with this, the graphs must have same degree of corresponding vertices. A quantity such that it has the same value for any graph belonging to the same isomorphic class is called an invariant. Hence the invariants are independent

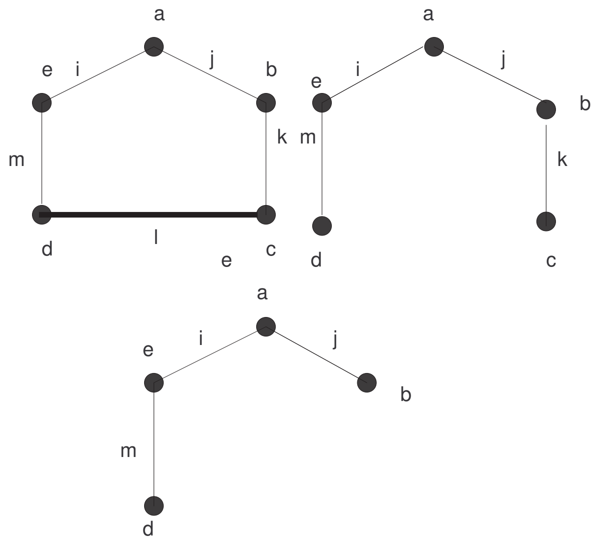

Figure 1.5: Deletion of an edge and vertex.

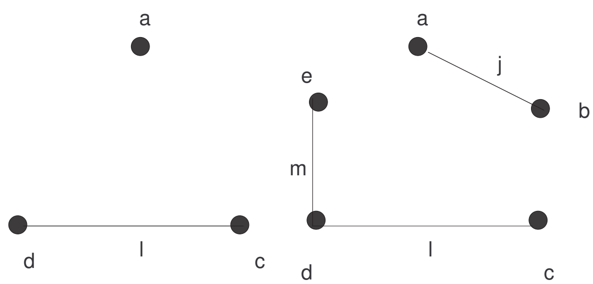

Figure 1.6: Edge-cut and vertex-cut.

of the vertex labeling and position. The isomorphic mapping of a graph onto itself such that the adjacency relationship is preserved is called automorphism. Each graph has atleast one automorphism, called the trivial automorphism or identity automorphism.

1.5 Special families of graphs

A graph that contains no cycles is called an acyclic graphs. An acyclic graph is called a forest. A tree is a set of straight line segments connected at their ends containing no closed loops, it is a simple, connected and acyclic graph. A forest is a graph such that all of its components are trees. A complete graph of order n is a simple graph in which

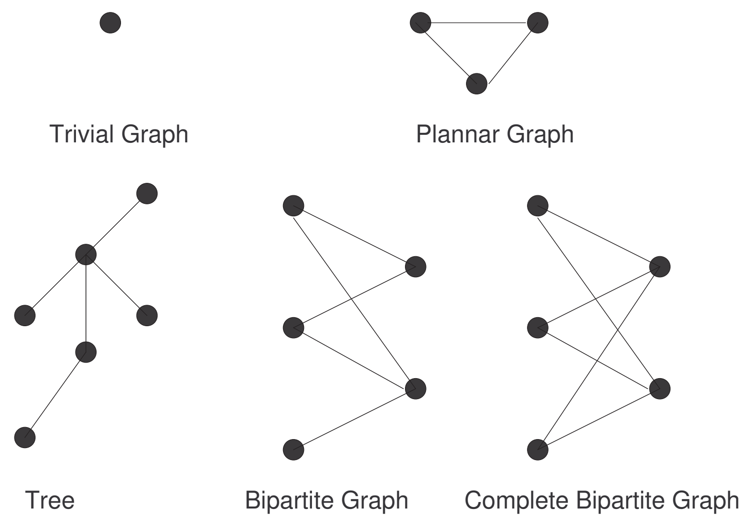

Figure 1.7: Basic families of graphs

any two vertices are connected by an edge. It is denoted by K_n. A bipartite graph G is a graph whose vertex set can be partitioned into two sets A and B with cardinalities m and n, respectively, such that every edge in G has one end vertex in A and other end-vertex in B. These sets A and B are called partite sets of G. A bipartite graph with partite sets A and B is called complete if for each vertex $x \in A$ and $y \in B$, there is an edge $xy \in E(G)$. If $|A| = r$ and $|B| = s$ then a complete bipartite graph with partite sets A and B is denoted by $K_{r,s}$. A star S_n is a graph that belongs to the family of trees. This is a graph such that it has n vertices, the degree of one of the vertices is $n-1$, where all the other vertices have degree 1.

Chapter 2

Chemical graph theory

In chemical graph theory, the graphs can represent a verity of chemical objects such as molecules, reactions, crystals, polymers, clusters, etc. The presence of sites and connection is common occurrence in such graphs. Sites which are usually called vertices may represent atoms, electrons, molecules, molecular fragments, groups of atoms, intermediates, orbitals, etc. The connections between these vertices represent bonds of any kind, which may range from a simple chemical bond to the steps of elementary actions, etc. Chemical graphs usually use a simple conversion rule: molecules or atoms as vertex and connection as edges. A special class of chemical graphs are molecular graphs. Molecular graphs also known as constitutional graphs are all structural formulas of covalently bounded compounds [1].

2.1 Graph invariants

Graph invariants have long been used in mathematical chemistry. These are the calculation based values as the experimentation takes alot of time. These invariants provide the chemists and mathematicians with valuable information regarding structural, physical, organic and medicinal chemistry [66]. Many of the old indicies, to this date, which are conceptually simple and computationally straightforward offer satisfactory structure-property-activity relations. They are very useful in QSARs and QSPRs studies [15, 31, 61, 63], some of these are path numbers of Platt, the Wiener number W, the path/walks shape indices of Randi and many others. The Wiener index is considered as the first non trivial index to be used in structure-property-activity [66]. These invariants continue to serve till this date and have produced some great work.

2.2 Zagreb and leap Zagreb indices

Another pair of important graph invariants are the Zagreb indices first introduced in [30] where the authors examined the dependence of total π-electron energy of molecular structures. For a molecular graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are, respectively, defined as follows.

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2 = \sum_{uv \in E(G)} (d_G(u) + d_G(v)), \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v). \quad (2.1)$$

The first and second Leap Zagreb indices are simply denoted by M_1 and M_2 respectively. A modification of the Zagreb indices such that second degree of vertices is considered was given in [7]. Leap Zagreb index is a degree based invariant. It is a fairly new index. The linear regression analysis of first leap Zagreb index with entropy, acentric factor, enthalpy of vaporization, standard enthalpy of vaporization and boiling point (BP) of octane isomers on the degree based topological indices of the corresponding molecular graphs was discussed in [11]. Some expressions regarding corona product, cartesian product, composition, disjunction and symmetric difference of graphs are given in [8]. Let G be a chemical graph then the first leap Zagreb index $LM_1(G)$, given by (2.2), is equal to the sum of squares of the second degrees of the vertices of G. The second Leap Zagreb index $LM_2(G)$, given by (2.3), is equal to the sum of the products of the second degrees of pairs of adjacent vertices in G. The third leap Zagreb index $LM_3(G)$, given by (2.4), is the sum of the products of the first degrees and second degrees of the vertices of G.

Mathematically, $LM_1(G)$, $LM_2(G)$ and $LM_3(G)$ are defined as follows.

$$LM_1(G) = \sum_{v\in V(G)} (d_G(v\,|\,2))^2 \tag{2.2}$$

$$LM_2(G) = \sum_{v\in V(G)} d_G(u)d_G(v\,|\,2) \tag{2.3}$$

$$LM_3(G) = \sum_{uv\in E(G)} d_G(u\,|\,2)d_G(v\,|\,2). \tag{2.4}$$

The leap Zagreb indices $LM_1(G)$, $LM_2(G)$ and $LM_3(G)$ are simply denoted as LM_1, LM_2 and LM_3, respectively.

2.3 Wiener index

Wiener is a distance based invariant with vast applications in the field of chemistry. It was introduced by Harold Wiener [20], in his study of effect of pure structural variation upon the boiling point of the paraffin. He called it path number and it is currently known as Wiener index $W(G)$ of a graph G. Platt [34] used the term Wiener number for it and the same has been exclusively used ever since. Wiener index is the most useful and one of the very first indices to be used in chemistry [17]. The use of modern topological indices in QSPR and QSAR was pioneered by the Wiener index. Mathematically, it is given by (2.5). Some more recent work has been done on the edge-Wiener index which obtains the distance between all pairs of the edge set. Explicit combinatorial expressions of these two edge-Wiener indices of some familiar graphs are discussed in [5].

In his study, he also introduced the concept of Wiener polarity index [20] denoted by $W_p(G)$. Hosoya [22] found a physical-chemical interpretation of $W_p(G)$. The Winer polarity index [20] is defined as the number of unordered pair of vertices such that they are at a distance 3 from each other.Mathematically $W_p(G)$ is given by (2.6). Some of the recent work on extremal Wiener polarity index of trees with different parameters is given in [32, 33]. It has helped in calculating the robustness of the system and also been used for lattice networks. Lukovits and Linert presented quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons by using Wiener polarity index [26]. The Wiener polarity index of fullerenes and hexagonal systems was studied in [6]. Recently, Arockiaraj et al. [51] studied the hyper-Wiener and Wiener polarity indices of silicate and oxide networks. Let G be a chemical graph representing the non-hydrogen atoms in the molecule. Then,

$$W(G) = \frac{1}{2}\sum_{l,m\in V} d_G(l,m) \tag{2.5}$$

$$W_p(G) = \big|\{\{u,v\} \subseteq V(G) \mid d_G(u,v)=3\}\big| = \frac{1}{2}\sum_{v\in V(G)} d_G(v\,|\,3). \tag{2.6}$$

Relation between Wiener polarity index and Zagreb indices was given by Liu and Liu [50]. They further discussed the second smallest Wiener polarity index among all trees of order n as well as smallest and second smallest Wiener polarity indices among all unicyclic graphs of order n. In 2018, Niko Tratnik [52] developed a method for computing the Wiener polarity index for most studied families of molecular graphs, benzenoid systems and carbon nanotubes. They further used the method to produce a formula for the Wiener polarity index applicable to any benzenoid system as well for zig-zag and armchair nanotubes.

2.4 Szeged index

A distance based graph invariant and some of its basic properties established in [23], till then no name had been given to the index, which became a nuisance for the researchers. In 1995 the index was named as Szeged index denoted by $Sz(G)$ [54]. Szeged index has been proved useful in the field of chemistry and biology. It has been useful in calculating molecular weight, densities, boiling points, vapor pressure, molar volume, molar refraction (MR), parachor, van der Waals volume, equalized electro-negativity, dipole moments, etc [67]. It has also provided valuable information in the field of biological sciences, by modeling various biological activities such as, anti-malarial, anti-tuberculotic, anti-HIV, etc [58].

We consider simple connected graphs such that e represents the edge between $u, v \in V$. Let $e = uv$ be an edge of G, connecting the vertices u and v. Then the sets N_u, N_v and N_0 are defined as the set of vertices of G lying closer to u than v, lying closer to v than u, and the set such that distance from u is same as the distance from v respectively. The cardinality of N_u, N_v and N_0 is given by $n_u(e)$, $n_v(e)$ and $n_0(e)$, respectively.

$$n_u(e) = |\{x \in V | d(x,u) < d(x,v)\}| \quad (2.7)$$

$$n_v(e) = |\{x \in V | d(x,u) > d(x,v)\}| \quad (2.8)$$

$$n_0(e) = |\{x \in V | d(x,u) = d(x,v)\}|. \quad (2.9)$$

For the edge $e = uv \in E$, we define the set M_u to be set of all edges $f \in E(G)$ such that the distance between f and the vertex u is less than the distance between f and v. The set M_v is the set of all edges $f \in E(G)$ such that the distance between f and the vertex v is less than the distance between f and u. Let M_0 denote the set of edges of G which are equi-distant from both u and v. The cardinality of M_u, M_v and M_0 is given by $m_u(e)$, $m_v(e)$ and $m_0(e)$ respectively.

$$m_u(e) = |\{f \in E \mid d(f,u) < d(f,v)\}| \quad (2.10)$$

$$m_v(e) = |\{f \in E \mid d(f,u) > d(f,v)\}| \quad (2.11)$$

$$m_0(e) = \{f \in E \mid d_G(f,u) = d_G(f,v)\}. \quad (2.12)$$

A variety of indices were designed to capture different aspects of molecular structure.The most popular is the Wiener index. The Wiener index of a connected graph G and its equivalent form for a tree T (see [20, 29])is defined in (2.13):

$$W = \sum_{e=uv \in E(T)} n_u(e) n_v(e) \quad (2.13)$$

Equation (2.13) is only valid when the graph in question is a tree. An index was needed for all the graphs. As a result the right hand-side of equation (2.13) was conceived as the Szeged index [23]. Notice that the atoms at equal distance were originally ignored in the definition. Szeged index attracted alot of attention but failed to produce satisfactory results in application to structure-property co-relations [66], as a result a modification was offered for the improvement of its performance. In this modification the vertices at equal distances were not ignored and given by (2.9). It was first proposed by Randić [39], who named it as revised Wiener index which was later named revised Szeged index in 2010 [66].

$$Sz^*(G) = \sum_{e\in E}\left(n_1(e) + \frac{n_0(e)}{2}\right)\left(n_2(e) + \frac{n_0(e)}{2}\right). \tag{2.14}$$

Later, Gutman and Ashrafi [25] introduced the edge version of Szeged index .

$$Sz(G) = \sum_{e\in E} m_1(e)m_2(e). \tag{2.15}$$

The revised-edge Szeged index was defined in [21] as:

$$Sz^*(G) = \sum_{e\in E}\left(m_1(e) + \frac{m_0(e)}{2}\right)\left(m_2(e) + \frac{m_0(e)}{2}\right). \tag{2.16}$$

Khalifeh et al. [43] defined the edge-vertex-Szeged index $Sz_ev(G)$ of a graph G as follows.

$$Sz_{ev}(G) = \frac{1}{2}\sum_{uv\in E(G)}(n_u(e)m_v(e) + n_v(e)m_u(e)). \tag{2.17}$$

The total-Szeged index was defined by Mahmiani et al. [9] as product of number of vertices and edges closer to one end-vertex of any edge and the other. That is,

$$Sz_t(G) = Sz(G) + Sz_e(G) + 2Sz_{ev}(G). \tag{2.18}$$

Some useful results in regards to the relationship between Szeged and Wiener index are given in the following theorem.

Theorem 2.1. [24] *Let G be a graph, then the Wiener index in general is smaller than the Szeged index, that is, $W(G) \leq Sz(G)$, where equality holds for complete graphs.*

Some of the more recent work in regards to the Szeged index on partial cubes and bounds of collected molecular graphs can seen in [40] and [35].After the success of Wiener and Szeged index a new index closely related to the two was introduced by Khadikar [59] called edge Padmakar-Ivan(PI) index. It has wide application in nano-technology.

$$PI(G) = \sum_{e \in E} m_1(e)m_2(e). \tag{2.19}$$

Chapter 3

The leap Zagreb indices of TiO_2 naotubes, 2-D lattices and nanotori

As a well-known semiconductor with numerous technological applications, titania nanotubes are comprehensively studied in materials science. Titania nanotubes were systematically synthesized during the last 10 to 15 years using different methods and carefully studied as prospective technological materials. The TiO_2 sheets with a thickness of a few atomic layers were found to be remarkably stable [60]. The graph of titanium nanotubes with m rows and n columns is denoted by $T_1(m, n)$ (see Figure 4.2). The 2-dimensional lattice obtained from titanium nanotubes $T_1(m, n)$ is denoted by $T_2(m, n)$ and is shown in Figure 4.2. In the same figure, we also present the titanium oxide nanotorus denoted by $T_3(m, n)$ obtained from $T_1(m, n)$. When m and n are obvious from the context, we denote the graphs $T_1(m, n)$, $T_2(m, n)$ and $T_3(m, n)$ by T_1, T_2 and T_3, respectively. The order and size of these graphs are given in Table 4.1.

First, we compute the Wiener polarity index of T_1, T_2 and T_3. For this purpose, we first define some notions related to the graphs $T_i(m, n)$, $i \in \{1, 2\}$. Using these notions, we will perform some necessary calculations which will then be summarized and presented in tables. For an n-vertex graph G, let $W_i = \{v \in V(G) \mid d_G(v \,|\, 3) = i\}$ for $1 \leq i \leq n-3$. Thus $W_1, W_2, \ldots, W_k$ is a vertex partitions of G, for some $k \in \{1, 2, \ldots, n-3\}$. The

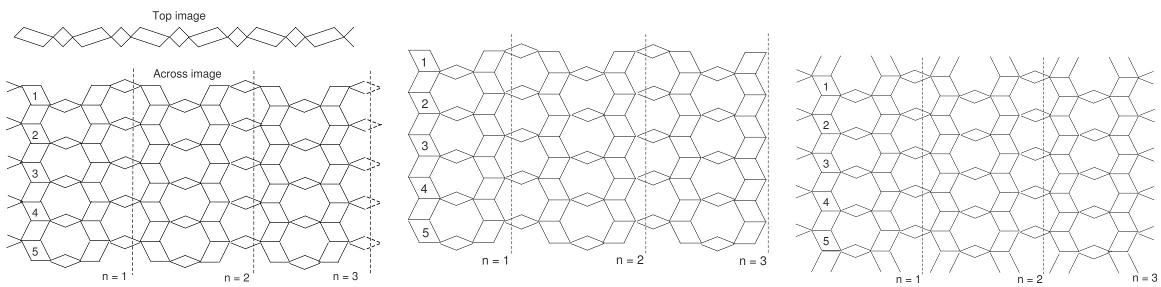

Figure 3.1: The graph on the left represents titania nanotube $T_1(5,3)$. The edges on the right are to be identified by the same edges on the left. The graph in the middle represents a 2-dimensional lattice denoted by $T_2(5,3)$ of titania nanotube. The graph on the right represents a nanotori $T_3(5,3)$. The edges on the right (resp., on the bottom) of nanotorus, are to be identified by the same edges on the left (resp., on the top)

The graph variant of TiO_2	order	size
$T_1(m,n)$	$12mn$	$4n(5m-1)$
$T_2(m,n)$	$2m(6n-1)$	$20mn-4(n+m)$
$T_3(m,n)$	$12mn$	$16n$ when $m=1$ and $20mn$ when $m \geq 2$

Table 3.1: The order and size of the graphs $T_1(m,n)$, $T_2(m,n)$ and $T_3(m,n)$ for $m \geq 1$ and $n \geq 1$.

vertex partition (W_i's) using third neighbors along with their cardinalities for the graphs $T_1(m,n)$, $T_2(m,n)$ and $T_3(m,n)$ are given in Tables 3.2-3.4.

i	$d_{T_1}(v\,|\,3)$	$|W_i|$
1	2	$8n$ when $m = 1$ and 0 when $m \geq 2$
2	4	$4n$ when $m = 1$, $12n$ when $m = 2$ and $8n$ when $m \geq 3$
3	5	0 when $m \leq 2$ and $4n$ when $m \geq 3$
4	6	0 when $m = 1$, $4n$ when $m = 2$ and $8n$ when $m \geq 3$
5	7	0 when $m \leq 2$ and $4n(m-3)$ when $m \geq 3$
6	8	0 when $m = 1$ and $4n(m-1)$ when $m \geq 2$
7	10	0 when $m \leq 2$, $4n$ when $m \geq 3$, $n = 1$ and 0 when $m \geq 3$, $n \geq 2$
8	11	0 when $m \leq 2$ and $4n$ when $m \geq 3$
9	14	0 when $m \leq 2$ and $4n$ when $m \geq 3$
10	15	0 when $m \leq 2$ and $4(m-3)$ when $m \geq 3$

Table 3.2: The cardinalities of the vertex partition W_i for the graph $T_1(m,n)$ with respect to the third neighbors of each vertex.

i	$d_{T_2}(v \mid 3)$	$\lvert W_i \rvert$
1	1	4 when $m = 1$ and 0 when $m \geq 2$.
2	2	$2(4n-1)$ when $m = 1$, 2 when $m = 2$ and 0 when $m \geq 3$
3	3	0 when $m = 1$ and 6 when $m \geq 2$.
4	4	$4(n-1)$ when $m = 1$, $4(3n-2)$ when $m = 2$ and $8n$ when $m \geq 3$
5	5	0 when $m = 1$, 2 when $m = 2$ and $2m + 4n - 8$ when $m \geq 3$
6	6	0 when $m = 1$, $4n + 2$ when $m = 2$ and $2m + 8n - 8$ when $m \geq 3$
7	7	0 when $m \in \{1, 2\}$, 4 when $m = 2$ and $4mn + 12n - 4m + 16$ when $m \geq 3$
8	8	$4(n-1)$ when $m \in \{1, 2\}$ and $4mn - 4n - 6$ when $m \geq 3$
9	10	$4(n-1)$ when $m \in \{1, 2\}$ and 2 when $m \geq 3$
10	11	0 when $m = 1$ and $2(m-2) + 2(2n-3)$ when $m \geq 3$
11	14	0 when $m \in \{1, 2\}$ and $4(n-1)$ when $m \geq 3$
12	15	0 when $m \in \{1, 2\}$ and $4(m-3)(n-1)$ when $m \geq 3$

Table 3.3: The cardinalities of the vertex partition W_i for the graph $T_2(m,n)$ with respect to the third neighbors of each vertex.

i	$d_{T_3}(v\,|\,3)$	$|W_i|$
1	2	$8n$ when $m=1$ and 0 when $m \geq 2$
2	4	$4n$ when $m=1$, $8n$ when $m=2$ and 0 when $m \geq 3$
3	6	0 when $m=1$ and $4mn$ when $m \geq 2$
4	8	0 when $m \leq 1$ and $4mn$ when $m \geq 3$
5	10	0 when $m=1$, $8n$ when $m=2$ and 0 when $m \geq 3$
6	14	0 when $m \leq 1$ and $4mn$ when $m \geq 3$

Table 3.4: The cardinalities of the vertex partition W_i for the graph $T_3(m,n)$ with respect to the third neighbors of each vertex.

In the following, we calculate the Wiener polarity index of graphs $T_1(m,n)$, $T_2(m,n)$ and $T_3(m,n)$ using Tables 3.3-3.4.

Theorem 3.1. *The Wiener polarity index for $T_1(m,n)$ is given by*

$$W_p(T_1(m,n)) = \begin{cases} 16n & m=1 \ \ and \ \ n \geq 1, \\ 72n & m=2 \ \ and \ \ n \geq 1, \\ 60mn-48n & m \geq 3 \ \ and \ \ n \geq 1. \end{cases} \tag{3.1}$$

Proof. Using the vertex partition W_i shown in Table 3.2, we have

$$W_p(T_1(m,n)) \;=\; \frac{1}{2}\sum_{w\in V(T_1)} |d_{T_1}(w\,|\,3)| = \frac{1}{2}\sum_{i=1}^{10} |N_{T_1}(w_i\,|\,3)|\cdot|W_i|.$$

We divide the proof in three cases.

Case 1: When $m=1$ and $n \geq 1$.

$$\begin{aligned} W_p(T_1(m,n)) \;&=\; \frac{1}{2}(2\cdot 8n + 4\cdot 4n + 5\cdot 0 + 6\cdot 0 + 7\cdot 0 + 8\cdot 0 + 10\cdot 0 + 11\cdot 0 + 14\cdot 0 \\ &\quad +15\cdot 0 = \frac{1}{2}(32n) = 16n. \end{aligned}$$

Case 2: When $m = 2$ and $n \geq 1$.

$$\begin{aligned} W_p(T_1(m,n)) &= \frac{1}{2}(2 \cdot 0 + 4 \cdot 12n + 5 \cdot 0 + 6 \cdot 4n + 7 \cdot 0 + 8 \cdot 4n + 10 \cdot 4n + 11 \cdot 0 + 14 \cdot 0 \\ &\quad +15 \cdot 0 \\ &= \frac{1}{2}(144n) = 72n. \end{aligned}$$

Case 3: When $m \geq 3$ and $n \geq 1$.

$$\begin{aligned} W_p(T_1(m,n)) &= \frac{1}{2}(2 \cdot 0 + 4 \cdot 8n + 5 \cdot 4n + 6 \cdot 8n + 7 \cdot 4n(m-3) + 8 \cdot 4n(m-1) + 10 \\ &\quad +11 \cdot 4n + 14 \cdot 4n + 15 \cdot 4n(m-3) = \frac{1}{2}(120mn - 96n) = 60mn - 48n. \quad \square \end{aligned}$$

Theorem 3.2. *The Wiener polarity index for $T_2(m,n)$ is given by*

$$W_p(T_2(m,n)) = \begin{cases} 16n - 8 & m = 1 \quad and \quad n \geq 1, \\ 72n - 30 & m = 2 \quad and \quad n \geq 1, \\ 60mn - 22m - 48n + 14 & m \geq 3 \quad and \quad n \geq 1, \end{cases} \tag{3.2}$$

Proof. Using the vertex partition W_i shown in Table 3.3, we get

$$W_p(T_2) = \frac{1}{2} \sum_{w \in V(T_2)} |d_{T_2}(w \,|\, 3)| = \frac{1}{2} \sum_{i=1}^{12} |N_{T_2}(w_i \,|\, 3)| \cdot |W_i|.$$

The proof is divided into three cases.

Case 1: When $m = 1$ and $n \geq 1$.

$$\begin{aligned} W_p(T_2(m,n)) &= \frac{1}{2}(1 \cdot 4 + 2 \cdot 2(4n-1) + 3 \cdot 0 + 4 \cdot 4(n-1) + 5 \cdot 0 + 6 \cdot 0 + 7 \cdot 0 + 8 \cdot 0 \\ &\quad +10 \cdot 0 + 11 \cdot 0 + 14 \cdot 0 + 15 \cdot 0 \\ &= \frac{1}{2}(32n - 16) = 16n - 8. \end{aligned}$$

Case 2: When $m = 2$ and $n \geq 1$.

$$\begin{aligned} W_p(T_2(m,n)) &= \frac{1}{2}(1 \cdot 0 + 2 \cdot 2 + 3 \cdot 6 + 4 \cdot 4(3n-2) + 5 \cdot 2 + 6 \cdot 4n + 2 + 7 \cdot 0 \\ &\quad +8 \cdot 4(n-1) + 10 \cdot 4(n-1) + 11 \cdot 0 + 14 \cdot 0 + 15 \cdot 0 \\ &= \frac{1}{2}(144n - 60) = 72n - 30. \end{aligned}$$

Case 3: When $m \geq 3$ and $n \geq 1$.

$$\begin{aligned} W_p(T_2(m,n)) &= \frac{1}{2}(1 \cdot 0 + 2 \cdot 0 + 3 \cdot 6 + 4 \cdot 8n + 5 \cdot (2m + 4n - 8) + 6 \cdot (2m + 8n - 8) \\ &\quad +7 \cdot (4mn - 12n - 4m + 16) + 8 \cdot (4mn - 4n - 6) + 10 \cdot 2 \\ &\quad +11 \cdot (2m + 4n - 10) + 14 \cdot 4(n-1) + 15 \cdot (4mn - m - 3n + 3) \\ &= \frac{1}{2}(120mn + 4m - 96n - 68) = 60mn + 2m - 48n - 34. \quad \square \end{aligned}$$

Theorem 3.3. *The Wiener polarity index for $T_3(m,n)$ is given by*

$$W_p(T_3(m,n)) = \begin{cases} 16n & m = 1 \quad \text{and} \quad n \geq 1, \\ 160n & m = 2 \quad \text{and} \quad n \geq 1, \\ 112mn & m \geq 3 \quad \text{and} \quad n \geq 1, \end{cases} \tag{3.3}$$

Proof. Consider the vertex partition W_i shown in Table 3.4. We have

$$W_p(T_3(m,n)) = \frac{1}{2} \sum_{w \in V(T_3)} |d_{T_3}(w, \mid 3)| = \frac{1}{2} \sum_{i=1}^{6} |N_{T_3}(w_i, \mid 3)| \cdot |V_i|.$$

The proof is divided into three cases.

Case 1: When $m = 1$ and $n \geq 1$.

$$\begin{aligned} W_p(T_3(m,n)) &= \frac{1}{2}(2 \cdot 8n + 4 \cdot 4n + 5 \cdot 0 + 6 \cdot 0 + 8 \cdot 0 + 8 \cdot 0 + 10 \cdot 0 + 14 \cdot 0 \\ &= \frac{1}{2}(32n) = 16n. \end{aligned}$$

Case 2: When $m = 2$ and $n \geq 1$.

$$\begin{aligned} W_p(T_3(m,n)) &= \frac{1}{2}(2 \cdot 0 + 4 \cdot 8n + 6 \cdot 8n \cdot 0 + 8 \cdot 0 + 10 \cdot 8n + 14 \cdot 0 \\ &= \frac{1}{2}(160n) = 80n. \end{aligned}$$

Case 3: When $m \geq 3$ and $n \geq 1$.

$$\begin{aligned} W_p(T_3(m,n)) &= \frac{1}{2}(2 \cdot 0 + 4 \cdot 0 + 6 \cdot 4mn + 8 \cdot 4mn + 10 \cdot 0 + 14 \cdot 4mn \\ &= \frac{1}{2}(112mn) = 56mn. \quad \square \end{aligned}$$

Next we compute the leap Zagreb index of first kind LM_1 of the graphs $T_1(m,n)$, $T_2(m,n)$ and $T_3(m,n)$. For an n-vertex graph G, let $V_i = \{v \in V(G) \mid d_G(v\,|\,2) = i\}$ for $1 \leq i \leq n-2$. Then $V_1, V_2, \ldots, V_k$ defines a vertex partitions of G, for some $k \in \{1, 2, \ldots, n-2\}$. This vertex partition along with the cardinalities of its partite sets for the graphs $T_1(m,n)$, $T_2(m,n)$ and $T_3(m,n)$ is given in Tables 3.5-3.7.

i	$d_{T_1}(v\,\|\,2)$	$\|V_i\|$
1	2	$4n$ when $m = 1$ and 0 when $m \geq 2$
2	3	0 when $m = 1$ and $4n$ when $m \geq 2$
3	4	0 when $m = 1$ and $4n$ when $m \geq 2$
4	5	$8n$ when $m = 1$ and $4n$ when $m \geq 2$
5	6	0 when $m = 1$ and $4n$ when $m \geq 2$
6	7	0 when $m = 1$ and $4n(m-1)$ when $m \geq 2$
7	9	0 when $m = 1$ and $4n$ when $m \geq 2$
8	10	0 when $m = 1$ and $4n(m-2)$ when $m \geq 2$

Table 3.5: The cardinalities of the vertex partition V_i for the graph $T_1(m,n)$ with respect to the second neighbors of each vertex, where $1 \leq i \leq 8$.

In the following, we compute the first type of leap Zagreb index of graphs $T_1(m,n)$, $T_2(m,n)$ and $T_3(m,n)$.

Theorem 3.4. *The leap Zagreb index for $T_1(m,n)$ is given by*

$$LM_1(T_1(m,n)) = \begin{cases} 1664n^2 & m = 1 \quad \text{and} \quad n \geq 1, \\ 2384m^2n^2 - 7968mn^2 + 9856n^2 & m \geq 2 \quad \text{and} \quad n \geq 1 \end{cases} \tag{3.4}$$

i	$d_{T_2}(v\,|\,2)$	$|V_i|$
1	1	2 when $m = 1$ and 0 when $m \geq 2$
2	2	$2(4n-1)$ when $m = 1$ and 2 when $m \geq 2$
3	3	4 when $m = 1$ and $4n$ when $m \geq 2$
4	4	0 when $m = 1$ and $4n + 2m - 2$ when $m \geq 2$
5	5	$8n - 6$ when $m = 1$ and $4mn - 4n - 2m + 4$ when $m \geq 2$
6	6	0 when $m = 1$ and $2m + 4n - 8$ when $m \geq 2$
7	7	0 when $m = 1$ and $4mn - 2m - 4n + 4$ when $m \geq 2$
8	8	0 when $m = 1$ and $2m - 4$ when $m \geq 2$
9	9	0 when $m = 1$ and $4n - 4$ when $m \geq 2$
10	10	0 when $m = 1$ and $4mn - 4m - 8n + 8$ when $m \geq 2$

Table 3.6: The cardinalities of the vertex partition V_i for the graph $T_2(m, n)$ with respect to the second neighbors of each vertex, where $1 \leq i \leq 10$.

Proof. For the vertex partition V_i $(1 \leq i \leq 8)$ shown in Table 3.5, we get

$$LM_1(T_1(m,n)) = \sum_{v \in V(T_1)} (d_{T_1}(v\,|\,2))^2 = \sum_{i=1}^{8} (|N_{T_1}(v_i\,|\,2)| \cdot |V_i|)^2.$$

There are two cases to be discussed.

Case 1: When $m = 1$ and $n \geq 1$, we have

$$\begin{aligned} LM_1(T_1(m,n)) &= (2 \cdot 4n)^2 + (3 \cdot 0)^2 + (4 \cdot 0)^2 + (5 \cdot 8n)^2 + (6 \cdot 0)^2 + (7 \cdot 0)^2 + (9 \cdot 0)^2 \\ &\quad + (10 \cdot 0)^2 \\ &= 1664n^2. \end{aligned}$$

i	$d_{T_3}(v\,|\,2)$	$|V_i|$
1	2	$4n$ when $m = 1$ and 0 when $m \geq 2$
2	4	0 when $m = 1$, $8n$ when $m = 2$ and 0 when $m \geq 3$
3	5	$8n$ when $m = 1$, $4mn$ when $m = 2$ and 0 when $m \geq 3$
4	7	0 when $m = 1$ and $4mn$ when $m \geq 2$
5	9	0 when $m = 1$, $8n$ when $m = 2$ and 0 when $m \geq 3$
6	10	0 when $m \leq 1$ and $4n$ when $m \geq 3$

Table 3.7: The cardinalities of the vertex partition V_i for the graph $T_3(m, n)$ with respect to the second neighbors of each vertex, where $1 \leq i \leq 6$.

Case 2: When $m \geq 2$ and $n \geq 1$, then

$$\begin{aligned} LM_1(T_1(m,n)) &= (2 \cdot 0)^2 + (3 \cdot 4n)^2 + (4 \cdot 4n)^2 + (5 \cdot 4n)^2 + (6 \cdot 4n)^2 + (7 \cdot 4n(m-1))^2 \\ &\quad + (9 \cdot 4n)^2 + (10 \cdot 4n(m-2))^2 = 2384m^2n^2 - 7968mn^2 + 9856n^2. \quad \square \end{aligned}$$

Theorem 3.5. *The leap Zagreb index for $T_2(m, n)$ is given by*

$$LM_1(T_2(m,n)) = \begin{cases} 1856n^2 - 2528n + 1064, & m = 1 \ \text{and} \ n \geq 1 \\ 2360m^2 - 4384m^2n + 8416mn + 2784m^2n^2 - 8768mn^2 & \\ +9856n^2 - 9888m + 8768mn - 20320n + 12288, & m \geq 2 \ \text{and} \ n \geq 1 \end{cases} \tag{3.5}$$

Proof. Using the information given in Table 3.6, we get

$$LM_1(T_2(m,n)) = \sum_{v \in V(T_2)} (d_{T_2}(v\,|\,2))^2 = \sum_{i=1}^{10} (|N_{T_2}(v_i\,|\,2)| \cdot |V_i|)^2.$$

The proof is divided into two cases.

Case 1: When $m = 1$ and $n \geq 1$.

$$\begin{aligned} LM_1(T_2(m,n)) &= (1 \cdot 2)^2 + (2 \cdot 2(4n-1))^2 + (3 \cdot 4)^2 + (4 \cdot 0)^2 + (5 \cdot 8n - 6)^2 + (6 \cdot 0)^2 \\ &\quad +(7 \cdot 0)^2 + (8 \cdot 0)^2 + (9 \cdot 0)^2 + (10 \cdot 0)^2 = 1856n^2 - 2528n + 1064. \end{aligned}$$

Case 2: When $m \geq 2$ and $n \geq 1$.

$$\begin{aligned} LM_1(T_2(m,n)) &= (1 \cdot 0)^2 + (2 \cdot 2)^2 + (3 \cdot 4)^2 + (4 \cdot 4n + 2(m-1))^2 + (5 \cdot 4mn - 4n \\ &\quad -2m + 4)^2 + (6 \cdot 2m + 4n - 8)^2 + (7 \cdot 2(2m-1) + 2(m-1)(2n-3)^2 \\ &\quad +(8 \cdot 2(m-2))^2 + (9 \cdot 4(n-1))^2 + (10 \cdot 4(m-2)(n-1)^2 \\ &= 2360m^2 - 4384m^2n + 8416mn + 2784m^2n^2 - 8768mn^2 + 9856n^2 \\ &\quad -9888m + 8768mn - 20320n + 12288. \quad \square \end{aligned}$$

Theorem 3.6. *The leap Zagreb index for $T_3(m,n)$ is given by*

$$LM_1(T_3(m,n)) = \begin{cases} 1664n^2, & m = 1 \quad and \quad n \geq 1 \\ 9344n^2 & m = 2 \quad and \quad n \geq 1 \\ 2784m^2n^2 & m \geq 3 \quad and \quad n \geq 1 \end{cases} \tag{3.6}$$

Proof. For the vertex partition V_i $(1 \leq i \leq 6)$ given in Table 3.7, we get the following.

$$LM_1(T_3(m,n)) = \sum_{v \in V(T_3)} (d_{T_3}(v\,|\,2))^2 = \sum_{i=1}^{6} (|N_{T_3}(v_i\,|\,2)| \cdot |V_i|)^2.$$

We complete the proof by considering the following three cases.

Case 1: When $m = 1$ and $n \geq 1$, then $LM_1(T_3(m,n)) = (2 \cdot 4n)^2 + (5 \cdot 8n)^2 = 1664n^2$.

Case 2: When $m = 2$ and $n \geq 1$, then $LM_1(T_3(m,n)) = (4 \cdot 8n)^2 + (7 \cdot 8n)^2 + (9 \cdot 8n)^2 = 9920n^2$.

Case 3: When $m \geq 3$ and $n \geq 1$, then $LM_1(T_3(m,n)) = (5 \cdot 4mn)^2 + (7 \cdot 4mn)^2 + (10 \cdot 4mn)^2 = 2784m^2n^2$. $\square$

Now, we compute the leap Zagreb indices of second and third kind (LM_2 and LM_3) for the graphs $T_1(m,n)$, $T_2(m,n)$ and $T_3(m,n)$. It can be seen from equation (2.2), (2.3) and (2.4) that leap Zagreb index $LM_2(G)$ and $LM_3(G)$ of a graph G can be computed by using an edge partition of G such that each edge $uv \in E(G)$ is contained in a unique partite set containing all edges whose end-vertices have second degrees $|N_G(u\,|\,2)|$ and $|N_G(v\,|\,2)|$. Let $\{V_1', V_2', \ldots, V_k'\}$ denotes such a partition for the graphs $T_1(m,n)$, $T_2(m,n)$ and $T_3(m,n)$. The cardinalities of V_i's are given in Tables 3.8-3.10.

i	$(d_{T_1}(u\,|\,2), d_{T_1}(v\,|\,2))$	$|V_i'|$
1	$(2,5)$	$16n$ when $m=1$ and 0 when $m \geq 2$
2	$(3,5)$	0 when $m \leq 2$ and $8n$ when $m \geq 3$
3	$(3,6)$	0 when $m=1$ and $4n$ when $m \geq 2$
4	$(3,9)$	0 when $m=1$ and $4n$ when $m \geq 2$
5	$(4,6)$	0 when $m=1$ and $4n$ when $m \geq 2$
6	$(4,7)$	0 when $m=1$ and $8n$ when $m \geq 2$
7	$(4,9)$	0 when $m=1$, $8n$ when $m=2$ and $4n$ when $m \geq 3$
8	$(4,10)$	0 when $m \leq 2$ and $4n$ when $m \geq 3$
9	$(5,7)$	0 when $m=1$ and $8n(m-2)$ when $m \geq 2$
10	$(5,9)$	0 when $m \leq 2$ and $4n$ when $m \geq 3$
11	$(5,10)$	0 when $m \leq 2$ and $4n(3m-7)$ when $m \geq 3$

Table 3.8: The cardinalities of the edge partition V_i' for the graph $T_1(m,n)$ with respect to the second neighbors of each vertex, where $1 \leq i \leq 11$.

In the following, we compute the leap Zagreb index of second and third kind (LM_2 and LM_3) of graphs $T_1(m,n)$, $T_2(m,n)$ and $T_3(m,n)$ by using Tables 3.8-3.10.

i	$(d_{T_2}(u\,|\,2), d_{T_2}(v\,|\,2))$	$\lvert V_i'\rvert$
1	$(1,3)$	4 when $m=1$ and 0 when $m\geq 2$
2	$(2,3)$	4 when $m=1$ and 0 when $m\geq 2$
3	$(2,4)$	0 when $m=1$ and 2 when $m\geq 2$
4	$(2,5)$	$4(4n-3)$ when $m=1$ and 2 when $m\geq 2$
5	$(3,4)$	0 when $m=1$ and 4 when $m\geq 2$
6	$(3,5)$	0 when $m=1$, $2(4n-1)$ when $m=2$ and $4(2n-1)$ when $m\geq 3$
7	$(3,6)$	0 when $m\leq 2$, $4(n-1)$ when $m=2$ and $2(2n-1)$ when $m\geq 3$
8	$(3,7)$	0 when $m=1$ and 4 when $m\geq 2$
9	$(3,9)$	0 when $m=1$ and $4(n-1)$ when $m\geq 2$
10	$(4,4)$	0 when $m=1$ and 2 when $m\geq 2$
11	$(4,5)$	$2(m-1)$ when $m\leq 2$ and 4 when $m\geq 3$
12	$(4,6)$	0 when $m=1$, $4(n-1)$ when $m=2$ and $4m-8+4n-6$ when $m\geq 3$
13	$(4,7)$	0 when $m=1$, $2(4n-1)$ when $m=2$ and $4(2n-1)$ when $m\geq 3$
14	$(4,8)$	0 when $m=1$ and $2(m-1)$ when $m\geq 2$
15	$(4,9)$	0 when $m=1$, $8(n-1)$ when $m=2$ and $4(n-1)$ when $m\geq 3$
16	$(4,10)$	0 when $m=1$ and $4(n-1)$ when $m\geq 2$
17	$(5,6)$	0 when $m=1$ and $2(m-2)$ when $m\geq 2$
18	$(5,7)$	0 when $m\leq 2$ and $8mn-16n-4m+10$ when $m\geq 3$
19	$(5,8)$	0 when $m\leq 2$ and $2(2m-5)$ when $m\geq 3$
20	$(5,9)$	0 when $m\leq 2$ and $4(n-1)$ when $m\geq 3$
21	$(5,10)$	0 when $m\leq 2$ and $4(3m-7)(n-1)$ when $m\geq 3$

Table 3.9: The cardinalities of the edge partition V_i' for the graph $T_2(m,n)$ with respect to the second neighbors of each vertex, where $1\leq i\leq 21$.

Theorem 3.7. *The leap Zagreb index for $T_1(m,n)$ is given by*

$$LM_2(T_1(m,n)) = \begin{cases} 112n, & m=1 \quad \textit{and} \quad n\geq 1 \\ 276mn-172n & m\geq 2 \quad \textit{and} \quad n\geq 1 \end{cases} \tag{3.7}$$

i	$(d_{T_3}(u\,|\,2), d_{T_3}(v\,|\,2))$	$\lvert V_i'\rvert$
1	$(2,5)$	$16n$ when $m=1$ and 0 when $m\geq 2$
2	$(5,7)$	0 when $m=1$ and $8mn$ when $m\geq 2$
3	$(5,9)$	0 when $m=1$, $24n$ when $m=2$ and 0 when $m\geq 3$
4	$(5,10)$	0 when $m\leq 2$ and $12mn$ when $m\geq 3$

Table 3.10: The cardinalities of the edge partition V_i' for the graph $T_3(m,n)$ with respect to the second neighbors of each vertex, where $1\leq i\leq 4$.

Proof. Let V_i' $(1\leq i\leq 11)$ be the edge partition given in Table 3.8. We compute the leap Zagreb index of second kind as follows.

$$\begin{aligned} LM_2(T_1(m,n)) &= \sum_{v\in V(T_1)} d(u)d(v\,|\,2) = \sum_{uv\in E(T_1)} (d(u\,|\,2)+d(v\,|\,2)), \\ &= \sum_{i=1}^{11} (|N_{T_1}(u_i\,|\,2)| + |N_{T_1}(v_i\,|\,2)|)\cdot |W_i|. \end{aligned}$$

The proof is divided into two cases.

Case 1: When $m=1$ and $n\geq 1$, then $LM_2(T_1(m,n)) = (2+5)\cdot 16n = 112n$.

Case 2: When $m\geq 2$ and $n\geq 1$, we get

$$\begin{aligned} LM_2(T_1(m,n)) &= (3+5)\cdot 8n + (3+6)\cdot 4n + (3+9)\cdot 4n + (4+6)\cdot 4n + (4+7)\cdot 8n \\ &\quad +(4+9)\cdot 4n + (4+10)\cdot 4n + (5+7)\cdot 8n(m-2) + (5+9)\cdot 4n \\ &\quad +(5+10)\cdot 4n(3m-7) \\ &= 276mn - 172n. \quad \square \end{aligned}$$

Theorem 3.8. *The leap Zagreb index for* $T_2(m,n)$ *is given by*

$$LM_2(T_2(m,n)) = \begin{cases} 112n-48, & m=1 \ \ \text{and} \ \ n\geq 1 \\ 276mn-90m-172n+42 & m\geq 2 \ \ \text{and} \ \ n\geq 1 \end{cases} \tag{3.8}$$

Proof. For the edge partition of the graph $T_2(m,n)$ given in Table 3.9. We get

$$\begin{aligned} LM_2(T_2(m,n)) &= \sum_{v\in V(T_2)} d(u)d(v\,|\,2) = \sum_{uv\in E(T_2)} (d(u\,|\,2)+d_2(v\,|\,2)), \\ &= \sum_{i=1}^{21} (|N_{T_2}(u_i\,|\,2)| + |N_{T_2}(v_i\,|\,2)|)\cdot |W_i|. \end{aligned}$$

The rest of the proof is divided into two cases.

Case 1: When $m=1$ and $n\geq 1$, then

$$\begin{aligned} LM_2(T_2(m,n)) &= ((1+3)\cdot 4) + ((2+3)\cdot 4) + ((2+5)\cdot 4(4n-3)) \\ &= 112n-48. \end{aligned}$$

Case 2: When $m\geq 3$ and $n\geq 1$, then

$$\begin{aligned} LM_2(T_2(m,n)) &= (2+4)\cdot 2 + (2+5)\cdot 2 + (3+4)\cdot 4 + (3+5)\cdot 4(2n-1) \\ &\quad +(3+6)\cdot 2(2n-1) + ((3+7)\cdot 4n) + (3+9)\cdot 4(n-1) + (4+4)\cdot 2 \\ &\quad +(4+5)\cdot 4 + (4+6)\cdot 4(m-2) + 2(2n-3) + (4+7)\cdot 4(2n-1) \\ &\quad +(4+9)\cdot 4(n-1) + (4+10)\cdot 4(n-1) + (5+6)\cdot 2(m-2) \\ &\quad +(5+7)\cdot (8n(m-2) - 2(2m-5)) + (5+8)\cdot 2(2m-5) \\ &\quad +(5+9)\cdot 4(n-1) + (5+10)\cdot 4(3m-7)(n-1) \\ &= 276mn - 90m - 172n + 42. \quad \square \end{aligned}$$

Theorem 3.9. *The leap Zagreb index for $T_3(m,n)$ is given by*

$$LM_2(T_3(m,n)) = \begin{cases} 112n, & m=1 \;\; \textit{and} \;\; n\geq 1 \\ 528n, & m=2 \;\; \textit{and} \;\; n\geq 1 \\ 276mn & m\geq 3 \;\; \textit{and} \;\; n\geq 1 \end{cases} \tag{3.9}$$

Proof. For the edge partition V_i' $(1\leq i\leq 4)$ given in Table 3.10, we compute the leap

Zagreb index of the graph T_3, as follows.

$$\begin{aligned} LM_2(T_3(m,n)) &= \sum_{v\in V(T_3)} d(u)d(v\,|\,2) = \sum_{uv\in E(T_3)} (d(u\,|\,2)+d(v\,|\,2)), \\ &= \sum_{i=1}^{4}(|N_{T_3}(u_i\,|\,2)|+|N_{T_3}(v_i\,|\,2)|)\cdot|W_i|. \end{aligned}$$

The proof is divided into three cases.

Case 1: When $m=1$ and $n\geq 1$, then $LM_2(T_3(m,n)) = (5+7)\cdot 16n+(5+9)\cdot 24n = 528n$.

Case 2: When $m=2$ and $n\geq 1$, then $LM_2(T_3(m,n)) = (2+5)\cdot 16n = 112n$.

Case 3: when $m\geq 3$ and $n\geq 1$, then $LM_2(T_3(m,n)) = (5+7)\cdot 8mn+(5+10)\cdot 12mn\cdot 4n) = 276mn$. □

Theorem 3.10. *The leap Zagreb index for $T_1(m,n)$ is given by*

$$LM_3(T_1(m,n)) = \begin{cases} 160n, & m=1 \quad and \quad n\geq 1 \\ 908n & m=2 \quad and \quad n\geq 1 \\ 880mn-856n & m\geq 3 \quad and \quad n\geq 1 \end{cases} \tag{3.10}$$

Proof. Consider the edge partition V_i' $(1\leq i\leq 11)$ given in Table 3.8. We compute LM_2 for the graph $T_3(m,n)$ as follows.

$$\begin{aligned} LM_3(T_1(m,n)) &= \sum_{u,v\in E(T_1)} d(u\,|\,2)d(v\,|\,2). \\ &= \sum_{i=1}^{11}((|N_{T_1}(u_i\,|\,2)|\cdot|N_{T_1}(v_i\,|\,2)|)\cdot|W_i|). \end{aligned}$$

There are three cases to be considered.

Case 1: When $m=1$ and $n\geq 1$, then $LM_3(T_1(m,n)) = (2\cdot 5\cdot 16)n = 160n$.

Case 2: When $m=2$ and $n\geq 1$, then

$$\begin{aligned} LM_2(T_1(m,n)) &= (3\cdot 5\cdot 8n)+(3\cdot 6\cdot 4n)+(3\cdot 9\cdot 4n)+(4\cdot 6\cdot 4n)+(4\cdot 7\cdot 8n) \\ &\quad +(4\cdot 9\cdot 8n) = 908n. \end{aligned}$$

Case 3: When $m \geq 3$ and $n \geq 1$, then we have

$$\begin{aligned} LM_2(T_1(m,n)) &= (3\cdot5\cdot8n)+(3\cdot6\cdot4n)+(3\cdot9\cdot4n)+(4\cdot6\cdot4n)+(4\cdot7\cdot8n) \\ &\quad +(4\cdot9\cdot4n)+(4\cdot10\cdot4n)+(5\cdot7\cdot8n(m-2))+(5\cdot9\cdot4n) \\ &\quad +(5\cdot10\cdot4n(3m-7)) = 880mn-856n. \quad \square \end{aligned}$$

Theorem 3.11. *The leap Zagreb index for $T_2(m,n)$ is given by*

$$LM_3(T_2(m,n)) = \begin{cases} 4(40n-21) & m=1 \ \ and \ \ n\geq 1 \\ 908n-410 & m=2 \ \ and \ \ n \geq 1 \\ 880mn-360m-856n+310 & m\geq 3 \ \ and \ \ n\geq 1. \end{cases} \tag{3.11}$$

Proof. For the edge partition V_i' $(1 \leq i \leq 21)$ given in Table 3.9, we have

$$\begin{aligned} LM_3(T_2(m,n)) &= \sum_{u,v\in E(T_2)} d_{T_2}(u\,|\,2)d_{T_2}(v\,|\,2). \\ &= \sum_{i=1}^{21}((|N_{T_2}(u_i\,|\,2)|\cdot|N_{T_2}(v_i\,|\,2)|)\cdot|W_i|). \end{aligned}$$

The proof is divided into three cases.

Case 1: When $m = 1$ and $n \geq 1$, then

$$LM_3(T_2(m,n)) = (1\cdot3\cdot4)+(2\cdot3\cdot4)+(2\cdot5\cdot4(4n-3)) = 4(40n-21).$$

Case 2: When $m = 2$ and $n \geq 1$, then we have

$$\begin{aligned} LM_3(T_2(m,n)) &= (2\cdot4\cdot2)+(2\cdot5\cdot2)+(3\cdot4\cdot4)+(3\cdot5\cdot2(4n-1)) \\ &\quad +(3\cdot6\cdot4(n-1))+(3\cdot7\cdot4)+(3\cdot9\cdot4(n-1))+(4\cdot4\cdot2) \\ &\quad +(4\cdot5\cdot2)+(4\cdot6\cdot4(n-1))+(4\cdot7\cdot2(4n-1))+(4\cdot9\cdot8(n-1)) \\ &= 908n-410. \end{aligned}$$

Case 3: When $m \geq 3$ and $n \geq 1$, then

$$\begin{aligned} LM_3(T_2(m,n)) &= (2\cdot 4\cdot 2)+(2\cdot 5\cdot 2)+(3\cdot 4\cdot 4)+(3\cdot 5\cdot 4(2n-1)) \\ &\quad +(3\cdot 6\cdot 2(2n-1))+(3\cdot 7\cdot 4)+(3\cdot 9\cdot 4(n-1))+(4\cdot 4\cdot 2) \\ &\quad +(4\cdot 5\cdot 4)+(4\cdot 6\cdot (4m-8+4n-6))+(4\cdot 7\cdot 4(2n-1)) \\ &\quad +(4\cdot 8\cdot 2(m-1))+(4\cdot 9\cdot 4(n-1))+(4\cdot 10\cdot 4(n-1)) \\ &\quad +(5\cdot 6\cdot 2(m-2))+(5\cdot 7\cdot (8mn-16n-4m+10))+(5\cdot 8\cdot 2(2m \\ &\quad -5))+(5\cdot 9\cdot 4(n-1))+(5\cdot 10\cdot 4(3mn-3m-7n+7)) \\ &= 880mn-360m-856n+310. \quad \square \end{aligned}$$

Theorem 3.12. *The leap Zagreb index for $T_3(m,n)$ is given by*

$$LM_3(T_3(m,n)) = \begin{cases} 160n, & m=1 \quad and \quad n\geq 1 \\ 1640n & m=2 \quad and \quad n\geq 1 \\ 880mn & m\geq 3 \quad and \quad n \geq 1 \end{cases} \tag{3.12}$$

Proof. Let V_i' $(1 \leq i \leq 4)$ represents the edge partition of the graph T_3 given in Table 3.10. We compute the leap Zagreb index of third kind for the graph T_3 as follows.

$$\begin{aligned} LM_3(T_3(m,n)) &= \sum_{u,v\in E(T_3)} d(u\,|\,2)d(v\,|\,2). \\ &= \sum_{i=1}^{4}((|N_{T_3}(u_i\,|\,2)|\cdot|N_{T_3}(v_i\,|\,2)|)\cdot|W_i|). \end{aligned}$$

We have the following three cases.

Case 1: When $m=1$ and $n\geq 1$, then $LM_3(T_3(m,n)) = (2\cdot 5\cdot 16) = 160n$.

Case 2: When $m=2$ and $n\geq 1$, then $LM_3(T_3(m,n)) = (5\cdot 7\cdot 16n)+(5\cdot 9\cdot 24n) = 1640n$.

Case 3: When $m\geq 3$ and $n \geq 1$, then $LM_3(T_3(m,n)) = (5\cdot 7\cdot 8mn)+(5\cdot 10\cdot 12mn) = 880mn$. $\square$

Chapter 4

Szeged-type indices of 2-dimensional lattices of TiO_2

4.1 Szeged-type indices of 2-dimensional lattices of TiO_2

In the next Section 4.1, we suggest such cuts which divides the graphs in two connected components which gives the values of n_u, n_v, m_u and m_v. Using these values we study several Szeged-type indices of 2-dimensional lattices of TiO_2

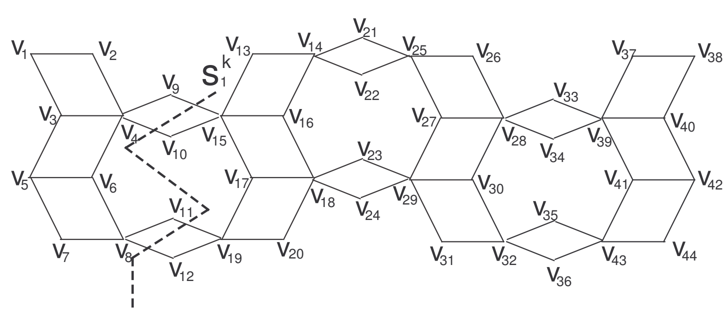

Figure 4.1: The graph represents the cuts suggested by Imran and Hafi [45].

In [45], the authors calculate the order and size of the titania nanotubes $T_1[m, n]$ to be $12mn$ and $20mn - 4n - 2m$, respectively. By comparing the formulas of order and size from Figure 4.2 and Table 4.1, it is clear that the formula for the size of titania nanotubes is not true. We denote the graph studied in [45] by $T_2'[m,n]$ (see Figure 4.2). Now consider the Θ-class denoted by S_1^k for titania nanotubes considered in [45] (see Figure 4.1). The edges in S_1^1 are $v_4v_{10}, v_9v_{15}, v_{11}v_{10}$ and v_8v_{12}. The values of m_u and m_v for these edges are $m_{v_9} = m_{v_4} = m_{v_{11}} = m_{v_8} = 13$ and $m_{v_{15}} = m_{v_{10}} = m_{v_{19}} = m_{v_{12}} = 51$. Whereas, for the graph of titania nanotubes considered in [45], the values of m_u and m_v obtained from definition (2.10) and (2.11) are given as follows:

$$m_{v_4} = 13, \quad m_{v_{10}} = 51,$$

$$m_{v_9} = 11, \quad m_{v_{15}} = 53,$$

$$m_{v_{11}} = 11, \quad m_{v_{19}} = 53,$$

$$m_{v_8} = 13, \quad m_{v_{12}} = 51.$$

Then the contribution of S_1^1 in computing the Szeged index of the graph $T_2'[m,n]$ is $4(13 \times 51)$ whereas all four edges in S_1^1 do not have the same values of m_1 and m_2. Thus the Szeged index calculated from S_1^1 is not correct in [45]. In this paper, we correct the results of [45] by defining new cuts for m_u and m_v for all edges $uv \in E(T_2[m,n])$

The graph variant of TiO_2	order	size
$T_1(m,n)$	$12mn$	$4n(5m-1)$
$T_2(m,n)$	$12mn - 2m$	$20mn - 4n - 4m$
$T_2'(m,n)$	$12mn$	$20mn - 4n - 2m$

Table 4.1: The order and size of the graphs $T_1(m,n)$, $T_2(m,n)$ and $T_3(m,n)$ for $m \geq 1$ and $n \geq 1$.

For the cut to be an orthognal cut it must contain all the edges such that they are equi-distant to each other. Let A_i, B_i, C_i, Y_i and Z_i be the types of edge-cuts of $T_2(m,n)$ as shown in Figure 4.3 and 4.4 by bold lines with negative slopes.Let A_i', B_i', C_i', Y_i'

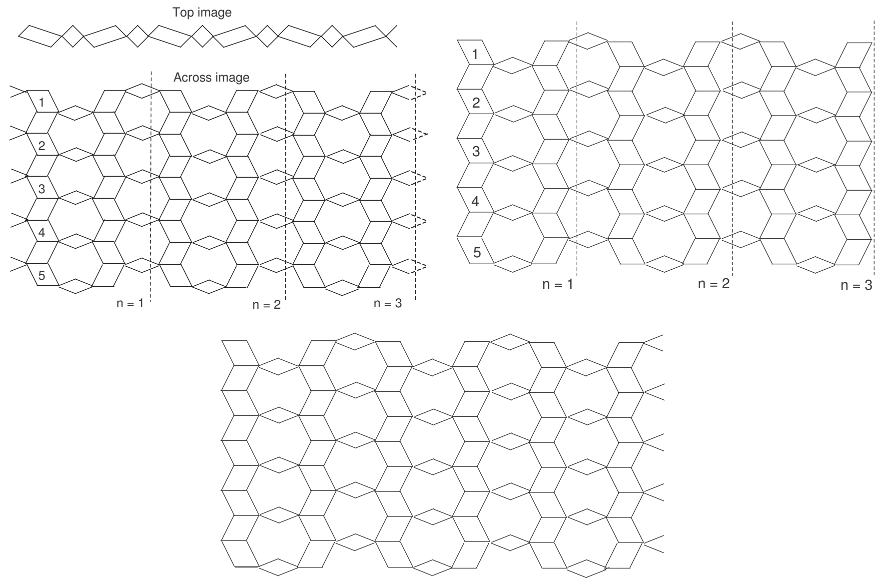

Figure 4.2: The graph on the left represents titania nanotube $T_1(5,3)$. The edges on the right, are to be identified by the same edges on the left. The graph in the middle represents a 2-dimensional lattice denoted by $T_2(5,3)$ of titania nanotube. The graph on the right studied in [45] represents a 2-dimensional lattice $T_2'(5,3)$ of titania nanotube.

and Z_i' denote the edge-cuts of the graph $T_2(m,n)$ obtained by reflecting the cuts A_i, B_i, C_i, Y_i and Z_i respectively. These cuts are denoted by thin dotted lines with positive slopes as shown in Figure 4.3 and 4.4. It is important to note that A_i, B_i, C_i and Y_i satisfy the definition of orthogonal cuts but the edge-cut Z_i is a simple cut such that the cut it contains all edges that satisfy the definition (2.12) and divides the graph in two components. The cardinality of the vertices and edges of these components provide the values of m_u, m_v, n_u, and n_v. Using these cuts we can evaluate the general formulas of the edges involved in each cut. It can be observed that there are $2n$ copies of a Y_i-type cuts and $2n-1$ copies of a Z_i-type cuts in $E(T_2(m,n))$, where the range of i can be obtained by varying m and n in $T_2(m,n)$.Then all the cuts of type A_i, B_i, C_i, Y_i and Z_i define a partition of $E(T_2(m,n))$. The number and sizes of these cuts are summarized in the following table 4.2.

When $m > n$, let $a_{1,e}$ and $a_{1,v}$ respectively denote the number of edges and vertices lying on one side of the cut A_1. Similarly, let $a_{i,e}$ and $a_{i,v}$, for $2 \leq i \leq n$, respectively denote the number of edges and vertices between the cuts A_i and A_{i-1}. Then $a_{i,e} = 4(4i-2)+1$ and $a_{i,v} = 4(3i-1)+1$, where $1 \leq i \leq n$. In the next theorem, we compute the

Case	cut-type	number of cuts	size of cuts
When $m > n$	A_i	$1 \leq i \leq n$	$4i$
	B_i	$1 \leq i \leq m-n-1$	$4n$
	C_i	$1 \leq i \leq n$	$2(2i-1)$
	Y_i	$1 \leq i \leq n$	$2m$
	Z_i	$1 \leq i \leq 2n-1$	$2m$
When $m \leq n$	A_i	$1 \leq i \leq m-1$	$4(4i-2)$
	B_i	$1 \leq i \leq n-m+1$	$4(m-1)+2$
	C_i	$1 \leq i \leq m-1$	$2(2i-1)$
	Y_i	$1 \leq i \leq n$	$2m$
	Z_i	$1 \leq i \leq 2n-1$	$2m$

Table 4.2: All types of edge-cuts in $T_2(m,n)$ with their cardinalities.

edge-Szeged index of the graph $T_2(m,n)$.

When $m \geq n$			When $m < n$		
type	range	size	type	range	size
$a_{i,e}$	$1 \leq i \leq n$	$4(4i-2)+1$	$a_{i,e}$	$1 \leq i \leq m$	$4(4i-2)+1$
$a_{i,v}$	$1 \leq i \leq n$	$4(3i-1)$	$a_{i,v}$	$1 \leq i \leq m$	$4(3i-1)$
$b_{i,e}$	$1 \leq i \leq m-n-1$	$4(4n-1)$	$b_{i,e}$	$1 \leq i \leq n-m+1$	$16m-2$
$b_{i,v}$	$1 \leq i \leq m-n-1$	$2(6n-1)$	$b_{i,v}$	$1 \leq i \leq n-m+1$	$12m$
$c_{i,e}$	$1 \leq i \leq n$	$4(4i-4)+1$	$c_{i,e}$	$1 \leq i \leq m$	$4(4i-4)+1$
$c_{i,v}$	$1 \leq i \leq n$	$2(6i-5)$	$c_{i,v}$	$1 \leq i \leq m$	$2(6i-5)$
$y_{i,e}$	$1 \leq i \leq n$	$2m(5i-4)-2i+1$	$y_{i,e}$	$1 \leq i \leq n$	$2m(5i-4)-2i+1$
$y_{i,v}$	$1 \leq i \leq n$	$2m(3i-2)$	$y_{i,v}$	$1 \leq i \leq n$	$2m(3i-2)$
$z_{i,e}$	$1 \leq i \leq 2n-1$	$2m(5i-2)-2i$	$z_{i,e}$	$1 \leq i \leq 2n-1$	$2m(5i-2)-2i$
$z_{i,v}$	$1 \leq i \leq 2n-1$	$2m(3i-1)+1$	$z_{i,v}$	$1 \leq i \leq 2n-1$	$2m(3i-1)+1$

Table 4.3: The number of vertices and edges lying between consecutive cuts of all types in the graph $T_2(m, n)$ with ranges and cardinalities.

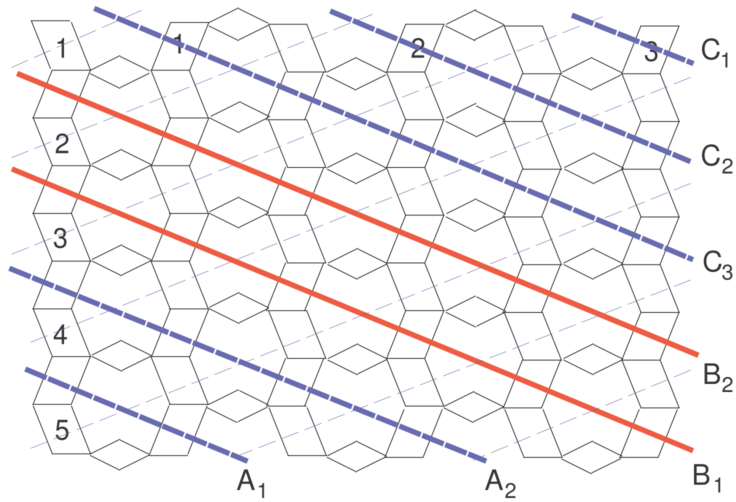

Figure 4.3: The edge-cuts of type A_i, B_i and C_i of the graph $T_2(m,n)$ for the case when $m \leq n$, where $m = 5$ and $n = 3$.

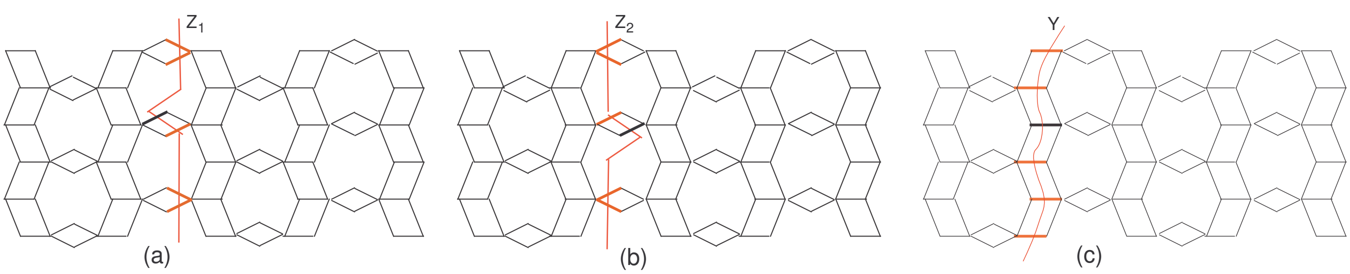

Figure 4.4: For $m = 3$ and $n = 2$, The edge-cuts of type Z_1, Z_2 and Y_i of the graph $T_2(m,n)$.

When $m > n$				
type	range	m_u	m_v	m_0
A_i	$1 \leq i \leq n$	$10i^2 - i$	$-10i^2 + 20mn - 3i - 4m - 4n$	$4i - 1$
B_i	$1 \leq i \leq m - n - 1$	$20in + 10n^2 - 4i - n$	$-20in + 20mn - 10n^2 + 4i$ $-4m - 7n$	$4n - 1$
C_i	$1 \leq i \leq n$	$-10i^2 + 20mn + 7i$	$10i^2 - 11i + 2 - 4m - 4n$	$2(2i - 1) - 1$
Y_i	$1 \leq i \leq n$	$10im - 2i - 8m + 1$	$-10im + 20mn + 2i + 2m - 4n - 1$	$2m - 1$
Z_i	$1 \leq i \leq 2n - 1$	$10im - 2i - 4m + 1$	$-10im + 20mn + 2i - 2m - 4n - 1$	$2m - 1$

When $m \leq n$				
type	range	m_u	m_v	m_0
A_i	$1 \leq i \leq m - 1$	$10i^2 - i$	$-10i^2 + 20mn - 3i - 4m - 4n$	$4i - 1$
B_i	$1 \leq i \leq n - m + 1$	$20im + 10m^2 - 4i$ $-21m + 4$	$-20im - 10m^2 + 20mn + 4i + 13m$ $-4n - 2$	$4m - 3$
C_i	$1 \leq i \leq m - 1$	$-10i^2 + 20mn + 7i$ $-4m - 4n$	$10i^2 - 11i + 2$	$2(2i - 1) - 1$
Y_i	$1 \leq i \leq n$	$10im - 2i - 8m + 1$	$-10im + 20mn + 2i + 2m - 4n - 1$	$2m - 1$
Z_i	$1 \leq i \leq 2n - 1$	$10im - 2i - 4m + 1$	$-10im + 20mn + 2i - 2m - 4n - 1$	$2m - 1$

Table 4.4: The values of m_u and m_v with respect to the cuts presented in Table 4.2 and the values presented in Table 4.3 for the graph T_2.

When $m > n$			
type	range	n_u	n_v
A_i	$1 \leq i \leq n$	$6i^2 + 2i - 1$	$-6i^2 + 12mn - 2i - 2m - 1$
B_i	$1 \leq i \leq m - n - 1$	$12in + 6n^2 - 2i + 2n - 1$	$-12in + 12mn - 6n^2 + 2i - 2m - 2n - 1$
C_i	$1 \leq i \leq n$	$-6i^2 + 12mn + 4i - 2m - 1$	$6i^2 - 4i - 1$
Y_i	$1 \leq i \leq n$	$2m(3i - 2) - 1$	$-6im + 12mn + 2m - 1$
Z_i	$1 \leq i \leq 2n - 1$	$6im - 2m$	$-6im + 12mn - 2$
When $m \leq n$			
type	range	n_u	n_v
A_i	$1 \leq i \leq n$	$6i^2 + 2i - 1$	$-6i^2 + 12mn - 2i - 2m - 1$
B_i	$1 \leq i \leq m - n - 1$	$12im + 6m^2 - 10m - 1$	$-12im - 6m^2 + 12mn + 8m - 1$
C_i	$1 \leq i \leq n$	$-6i^2 + 12mn + 4i - 2m - 1$	$6i^2 - 4i - 1$
Y_i	$1 \leq i \leq n$	$2m(3i - 2) - 1$	$-6im + 12mn + 2m - 1$
Z_i	$1 \leq i \leq 2n - 1$	$6im - 2m$	$-6im + 12mn - 2$

Table 4.5: The values of n_u and n_v with respect to the cuts presented in Table 4.2 and the values presented in Table 4.3 for the graph T_2.

Theorem 4.1. *The edge-Szeged index for 2-D lattice of TiO_2 nanotubes $T_2(m,n)$ for $m > n$ is given by,*

$$\begin{aligned} Sz_e(T_2(m,n)) &= -\left(\frac{2}{3}\right)n + 4m - \left(\frac{112}{3}\right)n^4 - \left(\frac{380}{3}\right)n^3 + \left(\frac{208}{3}\right)n^5 - \left(\frac{320}{3}\right)mn^4 \\ &\quad +448mn^3 - \left(\frac{2800}{3}\right)n^2m^3 + 272n^2m^2 + \left(\frac{4000}{3}\right)n^3m^3 - 960n^3m^2 \\ &\quad -32m^3 + \left(\frac{784}{3}\right)m^3n + 8m^2n - \left(\frac{92}{3}\right)mn - 8m^2 + \left(\frac{34}{3}\right)n^2. \end{aligned}$$

Proof. Let $T_2(m,n)$ be the graph of 2-dimensional lattice of TiO_2 nanotubes. Then for $m > n$ we calculate the edge-Szeged index by using Tables 4.2-4.4 as follows.

$$\begin{aligned} Sz_e(T_2(m,n)) &= 2(\sum_{i=1}^{n}((m_u)(m_v)(|A_i|)) + \sum_{i=1}^{m-n-1}((m_u)(m_v)(|B_i|)) + \sum_{i=1}^{n}((m_u)(m_v)(|C_i|)) \\ &\quad + \sum_{i=1}^{n}((m_u)(m_v)(|Y_i|)) + \sum_{i=1}^{2n-1}((m_u)(m_v)(|Z_i|))) \end{aligned}$$

$$\begin{aligned} Sz_e(T_2(m,n)) &= 2(\sum_{i=1}^{n}(10i^2 - i)(-10i^2 + 20mn - 3i - 4m - 4n)(4i) \\ &\quad + \sum_{i=1}^{m-n-1}(20in + 10n^2 - 4i - n)(-20in + 20mn - 10n^2 + 4i - 4m - 7n) \\ &\quad (4n) + \sum_{i=1}^{n}(10i^2 - 11i + 2)(-10i^2 + 20mn + 7i - 4m - 4n)(2(2i-1)) \\ &\quad + \sum_{i=1}^{n}(10im - 2i - 8m + 1)(-10im + 20mn + 2i + 2m - 4n - 1)(2m) \\ &\quad + \sum_{i=1}^{2n-1}(10im - 2i - 4m + 1)(-10im + 20mn + 2i - 2m - 4n - 1)(2m)) \end{aligned}$$

$$\begin{aligned} Sz_e(T_2(m,n)) &= -\left(\frac{2}{3}\right)n + 4m - \left(\frac{112}{3}\right)n^4 - \left(\frac{380}{3}\right)n^3 + \left(\frac{208}{3}\right)n^5 - \left(\frac{320}{3}\right)mn^4 \\ &\quad +448mn^3 - \left(\frac{2800}{3}\right)n^2m^3 + 272n^2m^2 + \left(\frac{4000}{3}\right)n^3m^3 - 960n^3m^2 \\ &\quad -32m^3 + \left(\frac{784}{3}\right)m^3n + 8m^2n - \left(\frac{92}{3}\right)mn - 8m^2 + \left(\frac{34}{3}\right)n^2. \end{aligned}$$

This completes the proof. □

Theorem 4.2. *The edge-Szeged index for $T_2(m,n)$ when $m \leq n$ is given by,*

$$\begin{aligned} Sz_e(T_2(m,n)) &= -\left(\frac{16}{3}\right)n - \left(\frac{32}{3}\right)n^3 - 176n^2m + \left(\frac{4000}{3}\right)n^3m^3 - 800n^3m^2 \\ &\quad -1360n^2m^3 + 752n^2m^2 + 160n^3m + 16m^4 - 64m^5 + \left(\frac{232}{3}\right)m^3 \\ &\quad +16n^2 + \left(\frac{880}{3}\right)m^4n + 16m^3n - \left(\frac{124}{3}\right)m^2n + \left(\frac{92}{3}\right)nm - 74m^2 \\ &\quad + \left(\frac{26}{3}\right)m. \end{aligned}$$

Proof. Let $T_2(m,n)$ be the graph of 2-dimensional lattice of TiO_2 nanotubes. Then for $m \leq$ we calculate the edge-Szeged index by using Tables 4.2-4.4 as follows.

$$\begin{aligned} Sz_e(T_2(m,n)) &= 2(\sum_{i=1}^{m-1}((m_u)(m_v)(|A_i|)) + \sum_{i=1}^{n-m+1}((m_u)(m_v)(|B_i|)) + \sum_{i=1}^{m-1}((m_u)(m_v)(|C_i|)) \\ &\quad + \sum_{i=1}^{n}((m_u)(m_v)(|Y_i|)) + \sum_{i=1}^{2n-1}((m_u)(m_v)(|Z_i|))) \end{aligned}$$

$$\begin{aligned} Sz_e(T_2(m,n)) &= 2(\sum_{i=1}^{m-1}((10i^2-i)(-10i^2+20mn-3i-4m-4n)(4i) + \sum_{i=1}^{n-m+1}(20im \\ &\quad +10m^2-4i-21m+4)(-20im-10m^2+20mn+4i+13m-4n \\ &\quad -2)(4(m-1)+2) + \sum_{i=1}^{m-1}(10i^2-11i+2)(-10i^2+20mn+7i-4m \\ &\quad -4n)(2(2i-1)) + \sum_{i=1}^{n}(10im-2i-8m+1)(-10im+20mn+2i+2m \\ &\quad -4n-1)(2m) + \sum_{i=1}^{2n-1}(10im-2i-4m+1)(-10im+20mn+2i-2m \\ &\quad -4n-1)(2m)) \end{aligned}$$

$$
\begin{aligned}
Sz_e(T_2(m,n)) &= -\left(\frac{16}{3}\right)n - \left(\frac{32}{3}\right)n^3 - 176n^2m + \left(\frac{4000}{3}\right)n^3m^3 - 800n^3m^2 \\
&-1360n^2m^3 + 752n^2m^2 + 160n^3m + 16m^4 - 64m^5 + \left(\frac{232}{3}\right)m^3 + 16n^2 \\
&+\left(\frac{880}{3}\right)m^4n + 16m^3n - \left(\frac{124}{3}\right)m^2n + \left(\frac{92}{3}\right)nm - 74m^2 + \left(\frac{26}{3}\right)m.
\end{aligned}
$$

This completes the proof. □

Theorem 4.3. *The vertex-Szeged index for $T_2(m,n)$ when $m > n$ is given by*

$$
\begin{aligned}
Sz_v(T_2(m,n)) &= 4 + \left(\frac{112}{15}\right)n - 160n^4 - \left(\frac{1104}{5}\right)n^5 - 96n^6 - 1248m^6 - \left(\frac{128}{3}\right)n^3 \\
&-4144m^4 - 352m^2 + 1936m^3 + 3792m^5 - 4m - \left(\frac{116}{3}\right)mn - 8304m^4n \\
&+5792m^3n - 1112m^2n + 4560m^3n^2 - 1536m^2n^2 + 3744m^5n - 480m^2n^3 \\
&+288mn^5 + 368mn^4 + 1248m^3n^3 - 3456m^4n^2 - 88mn^2 - \left(\frac{64}{3}\right)mn^3.
\end{aligned}
$$

Proof. Let $T_2(m,n)$ be the graph of 2-dimensional lattice of TiO_2 nanotubes. Then for $m > n$, we calculate the Szeged index by using Tables 4.2-4.5 as follows.

$$
\begin{aligned}
Sz_v(T_2(m,n)) &= 2\Big(\sum_{i=1}^{n}((n_u)(n_v)(|A_i|)) + \sum_{i=1}^{m-n-1}((n_u)(n_v)(|B_i|)) + \sum_{i=1}^{n}((n_u)(n_v)(|C_i|)) \\
&+\sum_{i=1}^{n}((n_u)(n_v)(|Y_i|)) + \sum_{i=1}^{2n-1}((n_u)(n_v)(|Z_i|))
\end{aligned}
$$

$$
\begin{aligned}
= \ & 2\Big(\sum_{i=1}^{n}(6i^2+2i-1)(-6i^2+12mn-2i-2m-1)(4i) + \sum_{i=1}^{m-n-1}(12in+6n^2-2i \\
&+2n-1)(-12in+12mn-6n^2+2i-2m-2n-1)(4n) + \sum_{i=1}^{n}(6i^2-4i-1)(-6i^2 \\
&+12mn+4i-2m-1)(2(2i-1)) + \sum_{i=1}^{n}(2m(3i-2)-1)(-6im+12mn+2m-1) \\
&(2m) + \sum_{i=1}^{2n-1}(6im-2m)(-6im+12mn-2)(2m)\Big).
\end{aligned}
$$

$$= 4+\left(\frac{112}{15}\right)n-160n^4-\left(\frac{1104}{5}\right)n^5-96n^6-1248m^6-\left(\frac{128}{3}\right)n^3-4144m^4-352m^2$$
$$+1936m^3+3792m^5-4m-\left(\frac{116}{3}\right)mn-8304m^4n+5792m^3n-1112m^2n+4560m^3n^2$$
$$-1536m^2n^2+3744m^5n-480m^2n^3+288mn^5+368mn^4+1248m^3n^3-3456m^4n^2$$
$$-88mn^2-\left(\frac{64}{3}\right)mn^3.$$

This completes the proof. □

Theorem 4.4. *The vertex-Szeged index for $T_2(m,n)$ when $m \leq n$ is given by,*

$$\begin{aligned} Sz_v(T_2(m,n)) &= -4n+48mn^2-96m^2n^3+480m^3n^3-240m^3n^2-192m^2n^2-48m^3n \\ &\quad +\left(\frac{80}{3}\right)m^4-\left(\frac{144}{5}\right)m^5+\left(\frac{40}{3}\right)m^3+80m^4n+104m^2n+4mn \\ &\quad -\left(\frac{80}{3}\right)m^2-\left(\frac{8}{15}\right)m. \end{aligned}$$

Proof. Let $T_2(m,n)$ be the graph of 2-dimensional lattice of TiO_2 nanotubes. Then for $m \leq n$, we calculate the Szeged index by using Tables 4.2-4.5 as follows.

$$\begin{aligned} Sz_v(T_2(m,n)) &= 2(\sum_{i=1}^{m-1}((n_u)(n_v)(|A_i|)) + \sum_{i=1}^{n-m+1}((n_u)(n_v)(|B_i|)) + \sum_{i=1}^{m-1}((n_u)(n_v)(|C_i|)) \\ &\quad + \sum_{i=1}^{n}((n_u)(n_v)(|Y_i|)) + \sum_{i=1}^{2n-1}((n_u)(n_v)(|Z_i|))) \end{aligned}$$

$$= 2(\sum_{i=1}^{m-1}(6i^2+2i-1)(-6i^2+12mn-2i-2m-1)(4i) + \sum_{i=1}^{n-m+1}(12im+6m^2$$
$$-10m-1)(-12im+12mn-6m^2+8m-1)(4(m-1)+2) + \sum_{i=1}^{m-1}(6i^2-4i-1)$$
$$(-6i^2+12mn+4i-2m-1)(2(2i-1)) + \sum_{i=1}^{n}(2m(3i-2)-1)(-6im+12mn$$
$$+2m-1)(2m) + \sum_{i=1}^{2n-1}(6im-2m)(-6im+12mn-2)(2m))$$

$$= -4n + 48mn^2 - 96m^2n^3 + 480m^3n^3 - 240m^3n^2 - 192m^2n^2 - 48m^3n + \left(\frac{80}{3}\right)m^4 - \left(\frac{144}{5}\right)m^5 + \left(\frac{40}{3}\right)m^3 + 80m^4n + 104m^2n + 4mn - \left(\frac{80}{3}\right)m^2 - \left(\frac{8}{15}\right)m.$$

This completes proof. □

Theorem 4.5. *The edge-vertex-Szeged index for $T_2(m,n)$ when $m > n$ is given by,*

$$\begin{aligned} Sz_{ev}(T_2(m,n)) &= \left(\frac{8}{15}\right)n - \left(\frac{110}{3}\right)mn + 4m + 112m^2n + \left(\frac{398}{3}\right)mn^2 + 84mn^3 \\ &\quad -20m^2 - 8m^3 + 800m^3n^3 - \left(\frac{1360}{3}\right)m^3n^2 - 288m^2n^3 - 144m^2n^2 \\ &\quad + \left(\frac{272}{3}\right)m^3n - \left(\frac{376}{3}\right)mn^4 + \left(\frac{752}{15}\right)n^5 + 10n^4 - \left(\frac{140}{3}\right)n^3 - 18n^2. \end{aligned}$$

Proof. Let $T_2(m,n)$ be the graph of 2-dimensional lattice of TiO_2 nanotubes. Then for $m > n$, we calculate the Szeged index by using Tables 4.2-4.5 as follows.

$$\begin{aligned} Sz_{ev}(T_2(m,n)) &= \sum_{i=1}^{n}((m_u)(n_v) + (m_v)(n_u))(|A_i|) + \sum_{i=1}^{m-n-1}((m_u)(n_v) + (m_v)(n_u))(|B_i|) \\ &\quad + \sum_{i=1}^{n}((m_u)(n_v) + (m_v)(n_u))(|C_i|) + \sum_{i=1}^{n}((m_u)(n_v) + (m_v)(n_u))(|Y_i|) \\ &\quad + \sum_{i=1}^{2n-1}((m_u)(n_v) + (m_v)(n_u))(|Z_i|) \end{aligned}$$

$$
\begin{aligned}
= \quad & \sum_{i=1}^{n}(-120i^4 + 240i^2mn - 52i^3 - 44i^2m - 24i^2n + 28imn - 4i^2 - 6im - 8in - 20mn \\
& +4i + 4m + 4n)(4i) + \sum_{i=1}^{m-n-1}(-480i^2n^2 + 480imn^2 - 480in^3 + 240mn^3 - 120n^4 \\
& +176i^2n - 176imn - 64in^2 - 16mn^2 - 76n^3 - 16i^2 + 16im + 28in - 26mn - 12n^2 \\
& +4m + 8n)(4n) + \sum_{i=1}^{n}(-120i^4 + 240i^2mn + 188i^3 - 44i^2m - 24i^2n - 212imn - 84i^2 \\
& +38im + 16in + 4mn + 12i + 4n - 2)(2(2i-1)) + \sum_{i=1}^{n}(-120i^2m^2 + 240im^2n \\
& +24i^2m + 120im^2 - 48imn - 176m^2n - 24im - 24m^2 + 8mn + 12m + 4n)(2m) \\
& + \sum_{i=1}^{2n-1}(-120i^2m^2 + 240im^2n + 24i^2m + 32im^2 - 48imn - 88m^2n - 36im + 4m^2 \\
& +20mn + 4i + 10m - 2)(2m)
\end{aligned}
$$

$$
\begin{aligned}
= \quad & \left(\frac{8}{15}\right)n - \left(\frac{110}{3}\right)mn + 4m + 112m^2n + \left(\frac{398}{3}\right)mn^2 + 84mn^3 - 20m^2 - 8m^3 \\
& +800m^3n^3 - \left(\frac{1360}{3}\right)m^3n^2 - 288m^2n^3 - 144m^2n^2 + \left(\frac{272}{3}\right)m^3n - \left(\frac{376}{3}\right)mn^4 \\
& + \left(\frac{752}{15}\right)n^5 + 10n^4 - \left(\frac{140}{3}\right)n^3 - 18n^2.
\end{aligned}
$$

This completes the proof. □

Theorem 4.6. *The edge vertex-Szeged index for $T_2(m, n)$ when $m \leq n$ is given by,*

$$
\begin{aligned}
Sz_{ev}(T_2(m,n)) \quad = \quad & 992m^3n^2 - 952m^2n^2 + 104mn^2 - 160m^6 + \left(\frac{2744}{5}\right)m^5 + 8n^2 \\
& - \left(\frac{5776}{3}\right)m^4n + 640m^5n + 16n^3 + \left(\frac{5924}{3}\right)m^3n - 726m^4 + \left(\frac{1406}{3}\right)m^3 \\
& + \left(\frac{548}{15}\right)m - 16mn^3 + 320m^2n^4 - 64mn^4 - \left(\frac{1748}{3}\right)m^2n + \left(\frac{160}{3}\right)mn \\
& -188m^2 + 480m^3n^3 - 368m^2n^3 - 480m^4n^2 - 4.
\end{aligned}
$$

Proof. Let $T_2(m, n)$ be the graph of 2-dimensional lattice of TiO_2 nanotubes. Then for $m \leq n$, we calculate the Szeged index by using Tables 4.2-4.5 as follows.

$$
\begin{aligned}
Sz_{ev}(T_2(m,n)) &= \sum_{i=1}^{m-1}((m_u)(n_v)+(m_v)(n_u))(|A_i|) + \sum_{i=1}^{n-m+1}((m_u)(n_v)+(m_v)(n_u))(|B_i|) \\
&\quad + \sum_{i=1}^{m-1}((m_u)(n_v)+(m_v)(n_u))(|C_i|) + \sum_{i=1}^{n}((m_u)(n_v)+(m_v)(n_u))(|Y_i|) \\
&\quad + \sum_{i=1}^{2n-1}((m_u)(n_v)+(m_v)(n_u))(|Z_i|)
\end{aligned}
$$

$$
\begin{aligned}
= &\sum_{i=1}^{m-1}(-120i^4+240i^2mn-52i^3-44i^2m-24i^2n+28imn-4i^2-6im-20mn+4i+4m \\
&+4n-8in)(4i) + \sum_{i=1}^{n-m+1}(-480i^2m^2-480im^3+480im^2n-120m^4+240m^3n+96i^2m \\
&+816im^2-96imn+384m^3-476m^2n-144im-334m^2+68mn+60m+4n-2)(4(m \\
&-1)+2) + \sum_{i=1}^{m-1}(-120i^4+240i^2mn+188i^3-44i^2m-24i^2n-212imn-84i^2+38im \\
&+16in+4mn+12i+4n-2)(2(2i-1)) + \sum_{i=1}^{n}(-120i^2m^2+240im^2n+24i^2m+120im^2 \\
&-48imn-176m^2n-24im-24m^2+8mn+12m+4n)(2m) + \sum_{i=1}^{2n-1}(-120i^2m^2 \\
&+240im^2n+24i^2m+32im^2-48imn-88m^2n-36im+4m^2+20mn+4i+10m \\
&-2)(2m)
\end{aligned}
$$

$$
\begin{aligned}
= \;& 992m^3n^2-952m^2n^2+104mn^2-160m^6+\left(\frac{2744}{5}\right)m^5+8n^2-\left(\frac{5776}{3}\right)m^4n \\
&+640m^5n+16n^3+\left(\frac{5924}{3}\right)m^3n-726m^4+\left(\frac{1406}{3}\right)m^3+\left(\frac{548}{15}\right)m-16mn^3 \\
&+320m^2n^4-64mn^4-\left(\frac{1748}{3}\right)m^2n+\left(\frac{160}{3}\right)mn-188m^2+480m^3n^3-368m^2n^3 \\
&-480m^4n^2-4.
\end{aligned}
$$

This completes the proof. □

Theorem 4.7. *The total Szeged index for $T_2(m,n)$ is given by,*

$$\begin{aligned}
Sz_t(T_2(m,n)) &= 4+\left(\frac{118}{15}\right)n+3744m^5n-8304m^4n+288mn^5-3456m^4n^2+3792m^5\\
&-\left(\frac{428}{3}\right)mn-880m^2n+\left(\frac{532}{3}\right)mn^2+\left(\frac{1784}{3}\right)mn^3+\left(\frac{12544}{3}\right)m^3n^3\\
&+2720m^3n^2-2016m^2n^3-1552m^2n^2+\left(\frac{18704}{3}\right)m^3n+\left(\frac{32}{3}\right)mn^4\\
&-4144m^4-1248m^6-96n^6-\left(\frac{532}{3}\right)n^4-\left(\frac{256}{5}\right)n^5+1888m^3-400m^2\\
&-\left(\frac{74}{3}\right)n^2-\left(\frac{788}{3}\right)n^3+8m, \quad \textit{if } m>n.\\
Sz_t(T_2(m,n)) &= -8-\left(\frac{28}{3}\right)n+1280m^5n-\left(\frac{10432}{3}\right)m^4n-960m^4n^2+\left(\frac{5024}{5}\right)m^5\\
&+\left(\frac{424}{3}\right)mn-\left(\frac{3308}{3}\right)m^2n+80mn^2+128mn^3+\left(\frac{8320}{3}\right)m^3n^3\\
&+384m^3n^2-1632m^2n^3-1344m^2n^2+\left(\frac{11752}{3}\right)m^3n-128mn^4\\
&-\left(\frac{4228}{3}\right)m^4-320m^6+640m^2n^4+1028m^3-\left(\frac{1430}{3}\right)m^2+32n^2\\
&+\left(\frac{64}{3}\right)n^3+\left(\frac{406}{5}\right)m, \quad \textit{if } m\le n.
\end{aligned}$$

Proof. To obtain the total Szeged index of $T_2(m,n)$ we divide the proof into following cases depending on the values of m and n :

Case 1: Using Theorems 4.1, 4.3 and 4.5, we calculate the total Szeged index for $m>n$, as follows.

$$
\begin{aligned}
Sz_t(T_2(m,n)) &= -\left(\frac{2}{3}\right)n+4m-\left(\frac{112}{3}\right)n^4-\left(\frac{380}{3}\right)n^3+\left(\frac{208}{3}\right)n^5-\left(\frac{320}{3}\right)mn^4\\
&\quad +448mn^3-\left(\frac{2800}{3}\right)n^2m^3+272n^2m^2+\left(\frac{4000}{3}\right)n^3m^3-960n^3m^2\\
&\quad -32m^3+\left(\frac{784}{3}\right)m^3n+8m^2n-\left(\frac{92}{3}\right)mn-8m^2+\left(\frac{34}{3}\right)n^24+\left(\frac{112}{15}\right)n\\
&\quad -160n^4-\left(\frac{1104}{5}\right)n^5-96n^6-1248m^6-\left(\frac{128}{3}\right)n^3-4144m^4-352m^2\\
&\quad +1936m^3+3792m^5-4m-\left(\frac{116}{3}\right)mn-8304m^4n+5792m^3n-1112m^2n\\
&\quad +4560m^3n^2-1536m^2n^2+3744m^5n-480m^2n^3+288mn^5+368mn^4\\
&\quad +1248m^3n^3-3456m^4n^2-88mn^2-\left(\frac{64}{3}\right)mn^3+\left(\frac{16}{15}\right)n-\left(\frac{220}{3}\right)mn\\
&\quad +8m+224m^2n+\left(\frac{796}{3}\right)mn^2+168mn^3-40m^2-16m^3+1600m^3n^3\\
&\quad -\left(\frac{2720}{3}\right)m^3n^2-576m^2n^3-288m^2n^2+\left(\frac{544}{3}\right)m^3n-\left(\frac{752}{3}\right)mn^4\\
&\quad +\left(\frac{1504}{15}\right)n^5+20n^4-\left(\frac{280}{3}\right)n^3-36n^2
\end{aligned}
$$

$$
\begin{aligned}
&= 4+\left(\frac{118}{15}\right)n+3744m^5n-8304m^4n+288mn^5-3456m^4n^2+3792m^5-\left(\frac{428}{3}\right)mn\\
&\quad -880m^2n+\left(\frac{532}{3}\right)mn^2+\left(\frac{1784}{3}\right)mn^3+\left(\frac{12544}{3}\right)m^3n^3+2720m^3n^2-2016m^2n^3\\
&\quad -1552m^2n^2+\left(\frac{18704}{3}\right)m^3n+\left(\frac{32}{3}\right)mn^4-4144m^4-1248m^6-96n^6-\left(\frac{532}{3}\right)n^4\\
&\quad -\left(\frac{256}{5}\right)n^5+1888m^3-400m^2-\left(\frac{74}{3}\right)n^2-\left(\frac{788}{3}\right)n^3+8m.
\end{aligned}
$$

Case 2: Using Theorems 4.2, 4.4 and 4.6, we calculate the total Szeged index for $m \le n$, as follows.

$$
\begin{aligned}
= \;& -\left(\frac{16}{3}\right)n-\left(\frac{32}{3}\right)n^3-176n^2m+\left(\frac{4000}{3}\right)n^3m^3-800n^3m^2-1360n^2m^3+752n^2m^2\\
&+160n^3m+16m^4-64m^5+\left(\frac{232}{3}\right)m^3+16n^2+\left(\frac{880}{3}\right)m^4n+16m^3n-\left(\frac{124}{3}\right)m^2n\\
&+\left(\frac{92}{3}\right)nm-74m^2+\left(\frac{26}{3}\right)m-4n+48mn^2-96m^2n^3+480m^3n^3-240m^3n^2\\
&-192m^2n^2-48m^3n+\left(\frac{80}{3}\right)m^4-\left(\frac{144}{5}\right)m^5+\left(\frac{40}{3}\right)m^3+80m^4n+104m^2n+4mn\\
&-\left(\frac{80}{3}\right)m^2-\left(\frac{8}{15}\right)m-8+1984m^3n^2-1904m^2n^2+208mn^2-320m^6+\left(\frac{5488}{5}\right)m^5\\
&+16n^2-\left(\frac{11552}{3}\right)m^4n+1280m^5n+32n^3+\left(\frac{11848}{3}\right)m^3n-1452m^4+\left(\frac{2812}{3}\right)m^3\\
&+\left(\frac{1096}{15}\right)m-32mn^3+640m^2n^4-128mn^4-\left(\frac{3496}{3}\right)m^2n+\left(\frac{320}{3}\right)mn-376m^2\\
&+960m^3n^3-736m^2n^3-960m^4n^2
\end{aligned}
$$

$$
\begin{aligned}
= \;& -8-\left(\frac{28}{3}\right)n+1280m^5n-\left(\frac{10432}{3}\right)m^4n-960m^4n^2+\left(\frac{5024}{5}\right)m^5+\left(\frac{424}{3}\right)mn\\
&-\left(\frac{3308}{3}\right)m^2n+80mn^2+128mn^3+\left(\frac{8320}{3}\right)m^3n^3+384m^3n^2-1632m^2n^3-1344m^2n^2\\
&+\left(\frac{11752}{3}\right)m^3n-128mn^4-\left(\frac{4228}{3}\right)m^4-320m^6+640m^2n^4+1028m^3-\left(\frac{1430}{3}\right)m^2\\
&+32n^2+\left(\frac{64}{3}\right)n^3+\left(\frac{406}{5}\right)m.
\end{aligned}
$$

This completes the proof. □

Theorem 4.8. *The Padmaker-Ivan index for $T_2(m,n)$ is given by,*

$$
\begin{aligned}
PI(T_2(m,n)) \;&=\; -\left(\frac{8}{3}\right)n+32mn+\left(\frac{32}{3}\right)n^3+400m^2n^2+24m^2-184m^2n-192mn^2\\
&\quad +32n^2,\ \text{if } m>n\\
PI(T_2(m,n)) \;&=\; 16n^2+400m^2n^2-160mn^2+\left(\frac{32}{3}\right)m^3+8m^2-216m^2n+64mn\\
&\quad +\left(\frac{16}{3}\right)m-8n,\quad \text{if } m\le n.
\end{aligned}
$$

Proof. Let T_2 be the graph of 2-dimensional lattice of TiO_2 nanotubes. Then for $m > n$ we calculate the Padmaker-Ivan index by using Tables 4.2-4.5 as follows.

$$\begin{aligned} PI(T_2(m,n)) &= 2(\sum_{i=1}^{n}((m_u)+(m_v))(|A_i|) + \sum_{i=1}^{m-n-1}((m_u)+(m_v))(|B_i|) + \sum_{i=1}^{n}((m_u)+(m_v))(|C_i|) \\ &\quad + \sum_{i=1}^{n}((m_u)+(m_v))(|Y_i|) + \sum_{i=1}^{2n-1}((m_u)+(m_v))(|Z_i|)) \end{aligned}$$

$$\begin{aligned} &= 2(\sum_{i=1}^{n}(((10i^2-i)+(-10i^2+20mn-3i-4m-4n))(4i) + \sum_{i=1}^{m-n-1}((20in+10n^2-4i \\ &\quad -n)+(-20in+20mn-10n^2+4i-4m-7n))(4n) + \sum_{i=1}^{n}((10i^2-11i+2)+(-10i^2 \\ &\quad +20mn+7i-4m-4n))(2(2i-1)) + \sum_{i=1}^{n}((10im-2i-8m+1)+(-10im+20mn \\ &\quad +2i+2m-4n-1))(2m) + \sum_{i=1}^{2n-1}((10im-2i-4m+1)+(-10im+20mn+2i-2m \\ &\quad -4n-1))(2m) \end{aligned}$$

$$\begin{aligned} &= 2(\sum_{i=1}^{n}(20mn-4i-4m-4n)(4i) + \sum_{i=1}^{m-n-1}(20mn-4m-8n)(4n) + \sum_{i=1}^{n}(20mn-4i \\ &\quad -4m-4n+2)(2(2i-1)) + \sum_{i=1}^{n}(20mn-6m-4n)(2m) + \sum_{i=1}^{2n-1}(20mn-6m-4n)(2m) \\ &= -\left(\frac{8}{3}\right)n + 32mn + \left(\frac{32}{3}\right)n^3 + 400m^2n^2 + 24m^2 - 184m^2n - 192mn^2 + 32n^2. \end{aligned}$$

Case 2: Let $T_2(m,n)$ be the graph of 2-D lattice of TiO_2 nanotubes. Then for $m \leq n$ we calculate the Padmaker-Ivan index by using Tables 4.2-4.5 as follows,

$$\begin{aligned} PI(T_2(m,n)) &= 2(\sum_{i=1}^{m-1}((m_u)+(m_v))(|A_i|) + \sum_{i=1}^{n-m+1}((m_u)+(m_v))(|B_i|) \\ &\quad + \sum_{i=1}^{m-1}((m_u)+(m_v))(|C_i|) + \sum_{i=1}^{n}((m_u)+(m_v))(|Y_i|) \\ &\quad + \sum_{i=1}^{2n-1}((m_u)+(m_v))(|Z_i|)) \end{aligned}$$

$$
\begin{aligned}
= \;& 2(\sum_{i=1}^{m-1}(((10i^2-i)+(-10i^2+20mn-3i-4m-4n))(4i)+\sum_{i=1}^{n-m+1}((20im+10m^2 \\
& -4i-21m+4)+(-20im-10m^2+20mn+4i+13m-4n-2))(4(m-1)+2) \\
& +\sum_{i=1}^{m-1}((10i^2-11i+2)+(-10i^2+20mn+7i-4m-4n))(2(2i-1))+\sum_{i=1}^{n}((10im \\
& -2i-8m+1)+(-10im+20mn+2i+2m-4n-1))(2m)+\sum_{i=1}^{2n-1}((10im-2i \\
& -4m+1)+(-10im+20mn+2i-2m-4n-1))(2m)
\end{aligned}
$$

$$
\begin{aligned}
= \;& 2(\sum_{i=1}^{m-1}(20mn-4i-4m-4n)(4i)+\sum_{i=1}^{n-m+1}(20mn-8m-4n+2)(4(m-1)2) \\
& +\sum_{i=1}^{m-1}(20mn-4i-4m-4n+2)(2(2i-1))+\sum_{i=1}^{n}(20mn-6m-4n)(2m) \\
& +\sum_{i=1}^{2n-1}(20mn-6m-4n)(2m)
\end{aligned}
$$

$$
= \; 16n^2+400m^2n^2-160mn^2+\left(\frac{32}{3}\right)m^3+8m^2-216m^2n+64mn+\left(\frac{16}{3}\right)m-8n.
$$

This completes proof $\square$

Theorem 4.9. *The revised edge-Szeged index for T_2 when $m > n$ is given by*

$$
\begin{aligned}
Sz_e^*(T_2) \;=\;& -\left(\frac{1}{2}\right)n+72m^3n+\left(\frac{3200}{3}\right)n^3m^3-\left(\frac{1600}{3}\right)n^2m^3-400n^3m^2-112n^2m^2 \\
& +134m^2n-16m^2-\left(\frac{220}{3}\right)n^3+\left(\frac{208}{3}\right)n^5-\left(\frac{640}{3}\right)mn^4+\left(\frac{448}{3}\right)mn^3 \\
& +\left(\frac{380}{3}\right)mn^2-52mn-2n^2+3m-12m^3
\end{aligned}
$$

Proof. Let T_2 be the graph of 2-dimensional lattice of TiO_2 nanotubes. Then for $m > n$ we calculate the revised edge-Szeged index by using Tables 4.2-4.5 as follows is given by:

$$
\begin{aligned}
Sz_e^*(T_2(m,n)) &= 2(\sum_{i=1}^{n}\left(m_u+\frac{m_0}{2}\right)\left(m_v+\frac{m_0}{2}\right))(|A_i|)+\sum_{i=1}^{m-n-1}\left(m_u+\frac{m_0}{2}\right)\left(m_v+\frac{m_0}{2}\right)(|B_i|) \\
&+\sum_{i=1}^{n}\left(m_u+\frac{m_0}{2}\right)\left(m_v+\frac{m_0}{2}\right)(|C_i|)+\sum_{i=1}^{n}\left(m_u+\frac{m_0}{2}\right)\left(m_v+\frac{m_0}{2}\right)(|Y_i|) \\
&+\sum_{i=1}^{2n-1}\left(m_u+\frac{m_0}{2}\right)\left(m_v+\frac{m_0}{2}\right)(|Z_i|))
\end{aligned}
$$

$$
\begin{aligned}
Sz_e^*(T_2(m,n)) &= 2(\sum_{i=1}^{n}-\frac{1}{4}(20i^2+2i-1)(20i^2-40mn+2i+8m+8n+1)(4i) \\
&+\sum_{i=1}^{m-n-1}-\frac{1}{4}(40in+20n^2-8i+2n-1)(40in-40mn+20n^2-8i \\
&+8m+10n+1)(4n)+\sum_{i=1}^{n}\left(10i^2-9i+\frac{1}{2}\right)(-10i^2+20mn+9i-4m \\
&-4n-\frac{3}{2})(2(2i-1))+\sum_{i=1}^{n}-\frac{1}{4}(20im-40mn-4i-6m+8n+3) \\
&(20im-4i-14m+1)(2m)+\sum_{i=1}^{2n-1}-\frac{1}{4}(20im-4i-6m+1)(20im \\
&-40mn-4i+2m+8n+3)(2m)
\end{aligned}
$$

$$
\begin{aligned}
Sz_e^*(T_2(m,n)) &= -\left(\frac{1}{2}\right)n+72m^3n+\left(\frac{3200}{3}\right)n^3m^3-\left(\frac{1600}{3}\right)n^2m^3-400n^3m^2 \\
&-112n^2m^2+134m^2n-16m^2-\left(\frac{220}{3}\right)n^3+\left(\frac{208}{3}\right)n^5-\left(\frac{640}{3}\right)mn^4 \\
&+\left(\frac{448}{3}\right)mn^3+\left(\frac{380}{3}\right)mn^2-52mn-2n^2+3m-12m^3
\end{aligned}
$$

This completes the proof. □

Theorem 4.10. *The revised edge-Szeged index for T_2 when $m \leq n$ is given by*

$$\begin{aligned} Sz_e^*(T_2(m,n)) &= -12 - \left(\frac{1147}{3}\right) n - \left(\frac{49}{3}\right) m + \left(\frac{7283}{3}\right) mn + \left(\frac{5200}{3}\right) n^5 \\ &+ \left(\frac{8000}{3}\right) m^4 n^2 - \left(\frac{26560}{3}\right) n^2 m^3 - 8800 n^3 m^3 + 10400 m^2 n^4 \\ &- \left(\frac{10400}{3}\right) mn^5 + 4900 n^3 + \left(\frac{15920}{3}\right) n^4 + 24000 m^2 n^3 - \left(\frac{47440}{3}\right) mn^4 \\ &+ \left(\frac{27232}{3}\right) m^2 n^2 - 19528 mn^3 - \left(\frac{14068}{3}\right) mn^2 - \left(\frac{3976}{3}\right) m^4 + 976 m^5 \\ &+ \left(\frac{2008}{3}\right) m^3 - \left(\frac{800}{3}\right) m^6 + 6764 m^3 n - 5848 m^2 n - 3520 m^4 n \\ &+ 800 m^5 n - 50 m^2 + \left(\frac{2884}{3}\right) n^2. \end{aligned}$$

Proof. Let $T_2(m,n)$ be the graph of 2-dimensional lattice of TiO_2 nanotubes. Then for $m \leq n$ we calculate the revised edge-Szeged index by using Tables 4.2-4.5 as follows,

$$\begin{aligned} Sz_e^*(T_2(m,n)) &= 2\Big(\sum_{i=1}^{m-1} \left(m_u + \frac{m_0}{2}\right)\left(m_v + \frac{m_0}{2}\right)\Big)(|A_i|) + \sum_{i=1}^{n-m+1} \left(m_u + \frac{m_0}{2}\right)\left(m_v + \frac{m_0}{2}\right)(|B_i|) \\ &+ \sum_{i=1}^{m-1} \left(m_u + \frac{m_0}{2}\right)\left(m_v + \frac{m_0}{2}\right)(|C_i|) + \sum_{i=1}^{n} \left(m_u + \frac{m_0}{2}\right)\left(m_v + \frac{m_0}{2}\right)(|Y_i|) \\ &+ \sum_{i=1}^{2n-1} \left(m_u + \frac{m_0}{2}\right)\left(m_v + \frac{m_0}{2}\right)(|Z_i|)\Big) \end{aligned}$$

$$
\begin{aligned}
Sz_e^*(T_2(m,n)) &= 2(\sum_{i=1}^{m-1} -\frac{1}{4}(20i^2+2i-1)(20i^2-40mn+2i+8m+8n+1)(4i) \\
&+ \sum_{i=1}^{n-m+1} -\frac{1}{4}(40in+20n^2-8i+2n-1)(40in-40mn+20n^2 \\
&-8i+8m+10n+9)(4m-2) + \sum_{i=1}^{m-1}\left(10i^2-9i+\frac{1}{2}\right) \\
&\left(-10i^2+20mn+9i-4m-4n-\frac{3}{2}\right)(2(2i-1)) + \sum_{i=1}^{n} -\frac{1}{4}(20im \\
&-4i-14m+1)(20im-40mn-4i-6m+8n+3)(2m) + \sum_{i=1}^{2n-1} -\frac{1}{4} \\
&(20im-4i-6m+1)(20im-40mn-4i+2m+8n+3)(2m)
\end{aligned}
$$

$$
\begin{aligned}
Sz_e^*(T_2(m,n)) &= -12-\left(\frac{1147}{3}\right)n-\left(\frac{49}{3}\right)m+\left(\frac{7283}{3}\right)mn+\left(\frac{5200}{3}\right)n^5 \\
&+\left(\frac{8000}{3}\right)m^4n^2-\left(\frac{26560}{3}\right)n^2m^3-8800n^3m^3+10400m^2n^4 \\
&-\left(\frac{10400}{3}\right)mn^5+4900n^3+\left(\frac{15920}{3}\right)n^4+24000m^2n^3-\left(\frac{47440}{3}\right)mn^4 \\
&+\left(\frac{27232}{3}\right)m^2n^2-19528mn^3-\left(\frac{14068}{3}\right)mn^2-\left(\frac{3976}{3}\right)m^4+976m^5 \\
&+\left(\frac{2008}{3}\right)m^3-\left(\frac{800}{3}\right)m^6+6764m^3n-5848m^2n-3520m^4n \\
&+800m^5n-50m^2+\left(\frac{2884}{3}\right)n^2.
\end{aligned}
$$

This completes proof. □

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