UNIVERSITI PUTRA MALAYSIA

COMPUTATION OF THREE TOPOLOGICAL INDICES ON SOME MOLECULAR GRAPHS AND FAMILIES OF NANOSTAR DENDRIMERS

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By

RAAD SEHEN HAOER

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for the Degree of Doctor of Philosophy

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DEDICATION

Every challenging work needs self efforts as well as guidance of elders especially those who were very close to our heart. Whose affection, love, encouragement and prays of day and night make me able to get such success and honor and the reason of what I become today.

My humble effort I dedicate to my sweet and loving

Father & Mother

To my brother and sisters, my wife and my kids (Mohammedali, Noorali and Mina)

I am really grateful to all of you.

You have been my inspiration, and my soul mates.

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirement for the degree of Doctor of Philosophy

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June 2018

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Chemical graph theory is a branch of mathematical chemistry which applies graph theory in mathematical modeling of chemical phenomena. One of the most active fields of research in chemical graph theory is the study of topological indices that can be used for describing and predicting physicochemical and pharmacological properties of organic compounds.

A topological index is a single unique number characteristic of the molecular graph and is mathematically known as the graph invariant. Eccentric connectivity Index, Zagreb-eccentricity indices and Wiener index are three of the most popular topological indices and used in wide spectrum of applications in chemical graph theory.

Motivated by the works done on characterization of mathematical properties for some nanostructures (dendrimers, nanotubes, nanotori, fullerenes etc.), we continue to investigate and obtain novelty formulas of the eccentric connectivity index for unicyclic chemical graph, chemical trees and some families of nanostar dendrimers. Also, we consider novelty formulas of the Zagreb-eccentricity indices for some families of nanostar dendrimers. Finally, novelty formulas for Wiener index of a new class of nanostar dendrimers are considered and new formulas associated with it are determined.

In this thesis, we study and analyses the molecular structures and structural properties of chemical compounds with the objective to represent them graphically and construct new classes of graphs. We use mathematical

methods of mathematical induction and mathematical logic to arrive at our theorems.

In particular, the Eccentric Connectivity Indices $\xi(G)$ are obtained for certain special graphs constructed by joining some special graphs to path graph. Through those graphs constructed are found $\xi(G)$ for graphs associated with some of molecular graphs such as chemical trees, chemical unicyclic graphs and some infinite families of nanostar dendrimers. Also, the Zagreb-eccentricity indices $Z(G)$ are found for some families of chemical trees, chemical unicyclic graphs and some infinite families of nanostar dendrimers. Finally, novel formulas for Wiener index of some dendrimers such as Polyphenelene dendrimers are established. Based on these investigations and graphical analysis novel formulas for the topological indices of these chemical compounds and nanotechnology are then obtained.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

PENGKOMPUTASIAN TIGA INDEKS TOPOLOGI BEBERAPA GRAF MOLEKULAR DAN FAMILI DENDRIMER NANOBINTANG

Oleh

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Teori graf kimia merupakan satu cabang tidang kimia bermatematik yang mengaplikasikan teori graf dalam pemodelan bermatematik fenomena kimia. Salah satu tumpuan bidang penyelidikan yang paling giat aijalankan dalam bidang teori graf kimia adalah pengkajian terhadap indeks topologi yang boleh digunakan untuk memperihalkan dan meramalkan sifat-sifat fisiokimia dan farmakologi sebatian organik.

Indeks topologi adalah suatu nombor unik yang tunggal yang mencirikan graf molecular yang dikenali dalam matematik sebagai ciri tak berubah grafitu. Indeks keberkaitan berpusat, indeks berpusat-Zagreb dan indeks Wiener merupakan tiga indeks topologi yang paling dikenali dan digunakan secara meluas aplikasinya dalam bidang teori graf.

Usaha penyelidikan yang dijalankan terhadap pencirian sifat-sifat matematik beberapa struktur nano (dendrimer, tiub nano, nanotori, fulleren dsb) telah menerbitkan minat dan motivasi dalam diri kami untuk menyelidik dan mendapatkan formula-formula baharu indeks keberkaitan berpusat bagi graf kimia unikitaran, pohon kimia dan beberapa keluarga dendrimer bintang nano. Kami juga cuba mendapatkan formula baru bagi indeks berpusat-Zagreb beberapa keluarge dendrimer bintang nano. Akhirnya, formula baru indeks Wiener suatu kelas baru dendrimer bintang nano dikaji dan formula baharnya diperoleh.

Dalam tesis ini, kami mengkaji dan menganalisis struktur molecular dan ciri-ciri struktur sebatian kimia dengan matlamat untuk menjelmakannya secara grafikal dan kemudian membina kelas-kelas baharu graf. Kami menggunakan kaedah induksi matematik dan juga kaedah mantik dalam bidang matematik untuk menghasilkan teorem-teorem yang berkaitan.

Khususnya, Indeks Keberkaitan Eksentrik $\xi(G)$ telah diperolehi bagi beberapa graf tertentu yang dibina dengan mencantumkan beberapa graf tertentu dengan graf lorong. Melalui graf yang dibina ini telah diperoleh $\xi(G)$ bagi graf yang disekutukan dengan beberapa graf molekular seperti graf pohon kimia, graf kimia unikitaran dan beberapa famili tak terhingga dendrimer nanobintang. Juga Indeks Keeksentrikan Zagreb Z(G) diperolehi bagi beberapa graf pohon kimia, graf kimia unikitaran dan beberapa famili yang tak terhingga dendrimer nanobintang. Akhir sekali rumusan indeks Weiner yang baharu bagi beberapa dendrimer seperti dendrimer Polifenelin telah dibangunkan. Berdasarkan penyelidikan ini dan cerakinan secara bergraf, rumusan baharu bagi indeks topologi sebatian-sebatian kimia dan teknologi nano tersebut telah diperolehi.

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This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philosophy.

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This is to confirm that:

- the research conducted and the writing of this thesis was under our supervision;
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LIST OF ABBREVIATIONS

G	The graph G
N	$\{0, 1, 2, 3, \dots\}$
$\|V\|$	The number of elements in the finite set V
$V(G)$	The vertex set of G
$E(G)$	The edge set of G
$deg(v)$	The number of edges incident on v
$N(v)$	Neighborhood of vertex v
T_n	The tree graph of order n
C_n	The cycle graph of order n
W_n	The wheel graph of order n
K_n	The complete graph of order n
$K_{m,n}$	The complete bipartite graph which one partite set has cardinality m and other partite set has cardinality n
$ECP(G)$	The eccentric connectivity polynomial of G
S_{n+1}	The star graph of order $n+1$
$d(x, y)$	The shortest distance between two vertices x and y in G
$\xi(G)$	The eccentric connectivity index of graph G
$ec(v)$	The length of a maximal path connecting v to another vertex of G
$W(G)$	The Wiener index of a graph G
$B_{n,d}$	The broom graph
$L_{n,d}$	The lollipop graph
$V_{n,d}$	The volcano graph
$G(m)$	The graph obtained from G by identifying the vertex V_0 of G with an end vertex y_0 of the path P_{m+1}
$G_1(m)G_2$	The graph obtained from adding a path P_m from a vertex in G_1 to a vertex of G_2
H_k	The molecular graph circumcoronene series of benzenoid
$T_{k,d}$	Some families of nanostar dendrimers
$NSB[n]$	An infinite family of nanostar dendrimer
$Z_1(G)$	The first Zagreb-eccentricity index of a graph G

$Z_2(G)$	The second Zagreb-eccentricity index of a graph G
$NSG[n]$	Type of nanostar dendrimers
$TPM[n]$	Type of nanostar dendrimer
$W_n^{P_r}$	The graph is constructed by joining the end- vertex of a path P_r to any vertex on the circumference of a wheel graph W_n
$F_n^{P_r}$	The graph is constructed by joining the end-vertex of a path to center vertex in the Fan graph
$K_{n,m}^{P_r}$	The graph is constructed by joining the end-vertex of a path to any terminal vertex of set vertices n in the complete bipartite graph
$(K_nK_m)^{P_r}$	The graph is constructed by joining each end-vertex of the path to any vertex of complete graph
$(W_nW_m)^{P_r}$	The graph is constructed by joining each end-vertex of a path to any vertex on the circumference of a wheel graph
$(F_nF_m)^{P_r}$	The graph is constructed by joining each end-vertex of the path to center vertex of Fan graph
$(K_{n,m}K_{a,b})^{P_r}$	The graph is constructed by joining each end-vertex of a path to any terminal vertex of sets vertices n and a in the two complete bipartite graphs
C_nH_{2n+2}	Molecular graphs representing the chemical compound of Alkanes
C_nH_{2n}	Molecular graphs representing the chemical compound of Alkenes
C_nH_{2n-2}	Molecular graphs representing the chemical compound of Alkynes
$C_n^{r_i}$	Unicyclic graph
C_n^{2n}	Molecular graphs representing the chemical compound of cycloalkanes
C_n^{2n-2}	Molecular graphs representing the chemical compound of cycloalkenes
C_n^{2n-2}	Molecular graphs representing the chemical compound of cycloalkynes
$AC_n^{R_i}$	Molecular graphs representing new classes of cycloalkanes
$EC_n^{R_i}$	Molecular graphs representing new classes of cycloalkenes

$YC_n^{R_i}$	Molecular graphs representing new classes of cycloalkynes
$PD[n]$	Polyther dendrimer
$PNS[n]$	Polymer Dendrimer
$PMD[n]$	PAMAM dendrimer
$PPD[n]$	Glutaroyl-AMINAP functionalised hyper branched dendrimer
$NSD[n]$	Type of Nanostar dendrimers
$G_1[n]$	Class of nanostar dendrimer
$G_2[n]$	Polyphenelene dendrimes
$B_r(G_2[n])$	A branch polyphenelene dendrimes

CHAPTER 1

INTRODUCTION

1.1 Motivation and Scope of the Study

Mathematical chemistry is a branch of theoretical chemistry using mathematical methods to discuss and predict molecular properties without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory in mathematical modelling of chemical phenomena. This theory has an important effect on the development of the chemical sciences. One of the most active fields of research in chemical graph theory is the study of topological indices that can be used for describing and predicting physicochemical and pharmacological properties of organic compounds. Also, the topological indices have many applications in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) to predict physico-chemical properties of chemical compounds (Kubiniy et al., 1999).

Topological indices are the numerical values associated with chemical constitution purporting for correlation of chemical structures with various physical properties, chemical reactivity or biological activity. The topological index of a molecule is a non-empirical numerical quantity that quantifies the structure and the branching pattern of the molecule. Therefore, the topological analysis of a molecule involves translating its molecular structure into a characteristic unique number (or index) that may be considered a descriptor of the molecule under examination. Such indices are widely used for establishing relationships between the structures of molecular graph and their physicochemical properties. The first use of a topological index for the correlation of the measured properties of molecules was made in 1947 by chemist Harry Wiener (Wiener, 1947).

Nowadays, there exists a legion of topological indices that found some applications in chemistry (Ritter & Wilson, 2000). They can be classified by the structural properties of graphs used for their calculation. Hence, The eccentric connectivity index (Sharma et al., 1997) and The Zagreb-eccentricity indices (Ghorbani & Hosseinzade, 2012) are based on the spectrum of the graph and the Wiener index (Wiener, 1947) are calculated using the distances of vertices, etc.

Topological indices, such as the Eccentric connectivity, Zagreb-eccentricity and Wiener indices are graph-theoretical invariants designed to find

relationships between the structure of chemical molecules and their physical properties. These indices have been used for isomer discrimination, chemical documentation, drug design, quantitative structure versus activity (or property) relationships (QSAR/QSPR's), combinatorial library design, and toxicology hazard assessments (Basak et al., 2000; Dureja et al., 2008; Lather & Madan, 2005c). This indices which have recently been employed successfully for the development of numerous mathematical models for the prediction of biological activities of diverse nature, have been reformed to overcome its limitations caused by degeneracy and insensitivity towards heteroatoms. Recently, a lot of results on the eccentric connectivity index has been obtained and some of them have been applied as means for modelling chemical, pharmaceutical and other properties of molecules, for details see (Gupta et al., 2002b; Gutman & Furtula, 2010; Sardana & Madan, 2001).

Nanotechnology refers to the engineering of functional systems at the nanoscale (Bhushan, 2010). A nanostructure is an object of bottom size of microscopic and molecular structures (Regan et al., 2005). A dendrimer is part of a new group of macromolecules that serve as photon funnels, similar to artificial antennas. This molecule is significantly resistant to photo bleaching. A dendrimer is an artificially manufactured or synthesized molecule built from branched units called monomers (Alikhani & Iranmanesh, 2010). Dendrimers have received considerable scientific interest because of their unique molecular architecture (Vögtle et al., 2009).

Through the above, the mathematical formulas above can be generalized to all special, molecular graphs and nanostar dendrimers in the same class. The results obtained in our research as presented will replace all above previous indices found by earlier researchers because these indices are difficult to calculate for more complicated structures. These mathematical formulas which give the numerical values associated with chemical constitution will give information on the correlation of chemical structures with various physical properties and chemical reactivity or biological activity. That is, the numerical values of these topological indices will help chemists to obtain description and prediction and further information on the physical and chemical properties for so many classes of chemical compounds and nanostar dendrimers.

Finally, in this thesis we introduce novelty general formulas for three topological indices such as the Eccentric connectivity, Zagreb-eccentricity and Wiener indices to certain special graphs, chemical compounds and families of dendrimers.

1.2 Basic Definitions and Notations

A graph $G = (V(G), E(G))$ or simply $G = (V, E)$ is a collection of non- empty finite *vertex set* $V(G)$ and *edge set* $E(G)$ ($E(G)$ can be an empty set). Each element of $V(G)$ is called a vertex of G and each element of $\{u, v\} \epsilon E(G)$ is an unordered pair called an edge of G where $u, v \in V(G)$. Let $e = uv$ is edge of G, then the vertices u and v are adjacent to each other. Graph G is said to be of *order* n if $|V(G)| = n$ and *size* m if $|E(G)| = m$. A sub graph H of graph G is a graph H where $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. A graph $G = (V, E)$ is directed if the edge set is composed of ordered vertex pairs. A loop is an edge whose endpoints are equal, that is, an edge joining a vertex to its self. A graph G has multiple edges if more than one edge is connected to the same pair of vertices. A simple graph has no loop and no a multiple edge.

A walk in a graph G is a sequence of vertices in a graph $(v_0, v_1, \dots, v_i)$ such that each adjacent pair (v_0, v_1), $(v_1, v_2) \dots, (v_{i-1}, v_i)$ serves as edges in G. A path is a walk with no repeated vertices. A path with n vertices is denoted by P_n. The *distance* $d(x, y)$ of two vertices x and y in G is the length of the shortest (x, y) path in G. The eccentricity of a vertex u in G is the largest distance between u and any other vertex of G. The maximum distance between any two vertices in G is the *diameter* of G. The minimum distance between any two vertices in G is the *radius* of G.

A graph G is connected if each pair of its vertices is connected by a path. A graph G is disconnected if it is not connected. A *cycle graph* is a graph consisting of a single cycle or a nontrivial closed path called a cycle. A cycle graph with n vertices is denoted by C_n. A *tree graph* is a connected graph without cycles. A tree with n vertices is denoted by T_n. The *complete graph* K_n of order n is a simple graph with n vertices in which every vertex is adjacent to all other vertices. A *bipartite graph* G is a graph with independent sets V_1 and V_2, where V_1 and V_2 are partitions of $V(G)$. A *complete bipartite graph* is a bipartite graph with partite (disjoint) sets $V_1$and V_2 possessing the added property in which every vertex of V_1 is adjacent to every vertex of V_2. Complete bipartite graphs are denoted by $K_{m,n}$, where $|V_1| = m$ and $|V_2| = n$. The bipartite graph $K_{1,n}$ is called a star graph, also denoted by S_{1+m}, and this star is a special of tree graph. A *wheel* is a graph with n vertices $(n \geq 4)$, denoted by W_n and formed by connecting a single vertex to all vertices of C_{n-1}.

In *chemical graphs*, each vertex represents an atom of the molecule, and covalent bonds between atoms are represented by the edge between the corresponding vertices. A connected graph with maximum vertex degree at most 4 is said to be a *molecular graph*. It is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. This shape

derived from a chemical compound is often called its molecular graph, and can be G path, a tree, or in general a graph. Its graphical representation may resemble a structural formula of some (usually organic) molecule (Trinajstic´, 1983). A tree in which the maximum vertex degree does not exceed 4 is said to be a *chemical tree*. A *vertex* of a graph is said to be *pendant* if its neighbourhood contains exactly one vertex. An *edge* of a graph is said to be *pendant* if one of its vertices is a pendant vertex. A *unicyclic graph* is a connected graph in which the number of edges equals the number of vertices. A *unicyclic chemical graphs* is the unicyclic graph that has no vertex with degree greater 4.

Dendrimers are a new class of polymeric materials. They are highly branched, mono-disperse macromolecules (Ashrafi & Mirzargar, 2008; Karbasioun & Ashrafi, 2009). The structure of these materials has a great impact on their physical and chemical properties. They are being investigated for possible uses in nanotechnology, gene therapy, and other fields. Carbon nanotubes are one of the most promising materials for use as an electron emission source owing to their substantial emission current at relatively low applied voltage in addition to their excellent mechanical and chemical stability (Ruying, 1987; Sharma et al., 1997).

The principal concept is to formulate and prove the theorems that are presented in this thesis, have been discussed in the standard book of graph theory (Gross & Yellen, 2005). Therefore, only important definitions and fundamental notations that are related to graph and nanostructures will be introduced in our discussion. Proofs of the theorems of the study will be presented in detail. References for detailed and substantive analyses of the proofs of related theorems will also be provided.

Quantitative structure−property relationship *(QSPR)* and quantitative structure−activity relationship *(QSAR)* studies use statistical models to compute physical, chemical, or biological properties of a chemical substance from its molecular structure, encoded in a numerical form with the aid of various descriptors.

In this thesis, all graphs considered are non-trivial connected simple graphs.

1.3 Objectives of Study

1. To establish the general formulas for the eccentric connectivity index of certain special graphs.
2. To obtain formulas for the eccentric connectivity and the Zagreb-eccentricity indices of molecular graphs such as trees and unicyclic chemical graphs.
3. To consider formulas for the eccentric connectivity and Zagreb-eccentricity indices of infinite families of polyther, polymer, PAMAM, Glutaroyl-AMINAP functionalized hyper branched PPI and $NS[n]$ dendrimers.
4. To study the Wiener index and establish formulas for new classes of nanostar dendrimers as polyphenelene dendrimers and $\mathrm{G}_1[\mathrm{n}]$.

1.4 Organization of Thesis

This thesis is organized into seven chapters.

Chapter 2 presents a detailed review on the studies of topological indices, especially the eccentric connectivity, Zagreb-eccentricity and Wiener indices that supports this work.

Chapter 3 provides the general formulas for the eccentric connectivity index of certain special graphs.

Chapter 4 presents the general formulas for the eccentric connectivity and the Zagreb-eccentricity indices of molecular graphs such as trees and unicyclic chemical graphs.

In Chapter 5, we obtain the formulas for the eccentric connectivity and Zagreb-eccentricity indices of infinite families of polyther, polymer, PAMAM, Glutaroyl-AMINAP functionalized hyper branched PPI and $NS[n]$ dendrimers.

Chapter 6 gives the general formulas for the Wiener indices of two infinite families of nanostar dendrimers by using cut-method.

Chapter 7 provides summary of the work done in the determination of eccentric connectivity indices, Zagreb-eccentricity indices and Wiener index for the families of dendrimers and molecular graphs. The conclusion and some open problems are also given for further study.

All the results, mentioned in this thesis, are closely related. More specifically, these findings include major objectives. The first one is finding the general formulas of the topological indices which are related to some special graphs that have never been examined in the previous studies. In addition, this includes finding new graphs that have certain properties and the topological indices that can be applied in some sciences such as chemistry. In addition to the early works that have been mentioned in this chapter, we will find the general formulas for some topological indices of nanotechnology that are of more complicated structure that have not been studied so far.

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