Structural Properties of Certain Molecular Graphs

By

Shahid Imran

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Structural Properties of Certain Molecular Graphs

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By

Shahid Imran

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Name	Registration Number
Shahid Imran	CIIT/FA14-BSM-017/LHR

Supervisor

Dr. Muhammad Hussain

Associate Professor, Department of Mathematics

COMSATS University Islamabad, Lahore Campus

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Final Approval

This report titled

Structural Properties of Certain Molecular Graphs

By

Shahid Imran

CIIT/FA14-BSM-017/LHR

Has been approved

For the COMSATS University Islamabad, Lahore Campus

External Examiner: ____________________________

Dr.

Supervisor: ____________________________
Dr. Muhammad Hussain
Department of Mathematics /CUI, Lahore Campus

HoD:__________________________________
Dr. Sarfraz Ahmad
Department of Mathematics, Lahore Campus

Declaration

I Shahid Imran registration number **CIIT/FA14-BSM-017/LHR** hereby declare that I have produced the work presented in this report, during the scheduled period of study.

Date: ______________

____

Shahid Imran

CIIT/FA14-BSMATH-017/LHR

Certificate

It is certified that Shahid Imran (**CIIT/FA14-BSM-017/LHR)** has carried out all the work related to this report under my supervision at the Department of Mathematics, COMSATS University Islamabad, Lahore Campus, and the work fulfills the requirement for award of BS degree.

Date: ____________________

Supervisor:

____
Dr. Muhammad
Hussain
Associate Professor

Head of Department:

____
Dr. Sarfraz Ahmad
Associate Professor
Department of Mathematics

DEDICATION

To

My Parents

ACKNOWLEDGEMENTS

First of all, I would like to thank Allah Almighty who is most Gracious, Merciful and without the help of whom nothing could be completed. All the words I know are not enough to my tribute to my respected parents who have been always pray for me to reach on valuable place. I feel great pleasure in expressing my profound and heartiest gratitude to my supervisor, Dr. Muhammad Hussain, for his indispensable guidance, deep consideration, valuable suggestions and active cooperation that enable me to complete my work successfully. Further, I also like to thank Dr. Sarfraz Ahmad HoD of Mathematics of COMSATS University Islamabad, Lahore campus for collaboration and inciting morally to do a standard research. I would like to thank Sir Maqsood Ahmad for their fruitful suggestions, proper guidance and kind cooperation during the period of my research work. Their excellent knowledge motivation and help combined to make my research experience worthwhile. I am thankful to Mr. Muhammad Azeem, and Hafiz M. Bilal who have been continuous helped me directly or indirectly during my research.

Shahid Imran
CIIT/FA14-BSM-017/LHR

Abstract

Let $G=(V,E)$ be asimple connected graph. The sets of vertices and edges of G are denoted by $V=V(G)$ and $E=E(G)$ respectively. In such a simple molecular graph, vertices represent atoms and edges represent bonds. In chemical graph theory, we have many invariant polynomials and topological indices for molecular graph. In this thesis we focus on the structure of molecular graph of Bakelite network. Morever the vertices having degrees $(2,2),(2,3)$ and $(3,3)$ gives the generalized form of count of edges in terms of m and n. The m in chemical structure represent the number of rows and n represent the number of column in Bakelite structure. In this thesis we compute the different indices such as Atom bond conecctivity ABC,Geometric arithmatic $G(A)$, Zagreb, Hyper Zagreb, Augmented Zagreb, Randic index and Harmonic indices of Bakelite network. Topological indices are real numerical parameter of a chemical structural networks and structural networks. These networks are characterize its topology and graph invariant. The topological indices like Randic, ABC, $G(A)$, are used to diagnose the bioactivity of chemical compounds. Actually these topological indices is designed by transforming a chemical structure into a numeric number.

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Chapter 1

Introduction

Introduction

Cheminformatics is a new subject which is a combination of chemistry, information science and mathematics. There is a considerable usage of graph theory in chemistry. Chemical graph theory is the topology branch of mathematics chemistry which implements graph theory to mathematical modeling of chemical occurrence. There is a lot of research which is done in this area in the last few decades. This theory contributes a major role in the field of chemical science. It studies quantitative structure activity (QSPR) relationship that are used to predict the biological activities and properties of chemical compounds. In QSPR study, physics, chemical properties and topological indices such as wiener index, szeged index, Randic index, zagreb index and ABC index are used to predict bioactivity of the chemical compounds. A topological index is a function $\sum$ to the set of real numbers, where $\sum$ is the set of finite simple graphs with property to $ToP(G) = ToP(H)$ if both G and H are isomorphic. There is alot of research which has been done on topological indices of different graph families so far, and is of much important due to their chemical significance.

A topological index is actually a numeric quantity associated with chemical constitution purporting for correlation of chemical structure with many physico-chemical properties, chemical reactivity or you can say the biological activity. Actually topological indices are designed on the ground of transformation of a molecular graph into a number which characterize the topological of that graph. Multiprocessor interconnection networks are often required to connect thousands of homogeneously replicates processor- many pairs, each of which is called a processing node . Instead of using a shared memory, all synchronization and communication between processing node for program execution is often done via message passing. Design and use of multiprocessor interconnection networks have recently drawn considerable attention due to the availability of inexpensive, powerfull microprocessor and memory chips [8].

The octagonal, toroidal polyhex and generalized prism networks has been recongnized and versatile interconnection networks for massively parallel computing. This is mainaly due to the fact that these families of networks have topologies which reflect the communication pattern of a wide variety of natural problems. Toroidal polyhex networks have recently received a lot of attention for their scalability to larger networks, as apposed to more complex networks such as hypercubes [10]. A graph $G(V,E)$ with vertex set V and edge set E is connected, if their exist a connection between any pair of vertices in G. A network is simply a connected graph having no multiple edges and loops. A chemical graph is a graph whose vertices denote atoms and edges denote bonds between that atoms of any understanding chemical structure. The degree of vertex is the number of vertices which are connected to that fixed vertex by the edges.In a chemical graph the degree of any vertex is at most 4. The distance between two vertices u and v is denoted as $d(u,v) = d_G(u,v)$ and is the length of shortest path between u and v is also called $u - v$ **geodesic**. The longest path between any two vertices is called $u - v$ **detour**.In this article ,G is consider to be network with vertex set $v(G)$ and edge set $E(g)$, d_u is the degree of vertex $u \in V(G)$. The concept of topological index came from work done by **Harold Wiener** in 1947 while he was working on boiling point of paraffin. He named this index as path number. Later on, path number was renamed as **Wiener** index and then theory of topological index is started.

Chapter 2

Graph Theory

2.1 History:

The credit of beginning of graph theory goes to famous swiss mathematian named **Leonhard Euler** in 1735. Euler tried to solve the problem of Konigsbrerg brige. This problem was actuallya puzzle which was concerning for the possibility of finding the path using each one of the seven bridge that were made over a river flowing through an Island in Russia. The history of graph theory and topolog are closely related, and the two areas share common problems and techniques. Euler referred to his work on the Konigsberg bridge problem as an example of geometria situs-the “geometry of position”- while the development of topological ideas during the second half of the 19th century became known as analysis situs- the “Analysis of position”

The connection between the graph theory and topology led to subfield called topological graph theory. An important problem in this area concern planar graph. These are graph that can be drawn as dot-and-line diagram on a plane without any edges crossing except at the vertices where they meet. The use of diagram of dots and lines to represent graphs actually grew out of the 19th-century chemistry, where lettered vertices denoted individual atoms and connecting lines denoted chemical bonds..

2.2 Basic Definitions:

2.2.1 Graph:

Graph is a collection of vertices and edges that join pairs of vertices. The number of vertices in a graph G is called its order. The number of edges in a graph G is called its size. Multiedges graphs is called multigraphs. An edge that joins a vertex to itself is called a loop. A graph with no loop and multiple edges is called a simple graph.

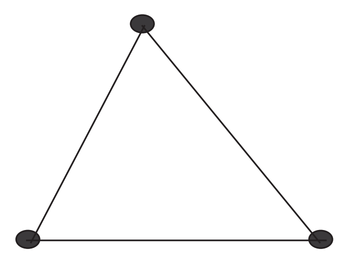

Figure 2.1: The simple graph

2.2.2 Path:

A walk is called path if all of its vertices are distinct.

2.2.3 Trail:

A walk is called trail if all of its edges are distinct.

2.2.4 Length of Walk:

Number of edge in a walk is called the length of a walk.

2.2.5 Closed Walk:

A walk in a graph G is called closed walk if $v_0 = v_n$.

2.2.6 Open Walk:

A walk in a graph G is not closed is called open walk.

2.2.7 Cycle:

A cycle is a path that consists of a sequence of vertices starting and ending on some vertex, with no repetitions of vertices and edges allowed.

2.2.8 Adjancy:

Two vertices say V and W joined by an edge are called Adjacent vertices and two edges say e and f are adjacent edges if they have a vertex in common.

2.2.9 Incident Vertices / Edeges

If $e = xy$ is en edge then we say that the vertices x and y are incident to e and e is incident to both x and y.

2.3 Types of Graph:

2.3.1 Planar Graph:

In graph theory, a planar graph is a graph that can be embedded in the plane. i.e it can be drawn on the plane in such a way that its edges intersect only at their end points. In other words, it can be drawn in such a way that no edges cross each other.

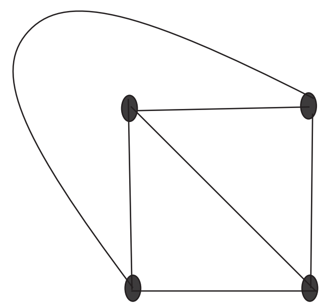

Figure 2.2: The planar graph

2.3.2 Non-planar Graph:

A graph G which can not be embedded in the plane is called non-planar.

2.3.3 Finite Graph:

G is called finite if the sets V_G and E_G having finite cardinality.

2.3.4 Order/Size of Graph:

The cardinality of set V_G in a graph is called the order of G. The cardinality of set E_G in a graph is called the size of G.

2.3.5 Multi Graph:

In mathematics and more specially in graph theory, a multi graph (in contrast a simple graph) is a graph which is permitted to have multi edges (also called parallel edges), that is, edges that have the same end nodes. Thus two vertices may be connected by more than one edge.

2.3.6 Bipartite Graph:

A bipartite graph G is a graph in which $V(G)$ can be partitioned in two sets a and b such that a and b no two vertices are adjacent.

2.3.7 Sub-divided Graph:

In a graph G, if inserting at least one new vertex in each edge then we obtain a sub-divided graph.

2.3.8 Null graph

Let G be a graph. The null graph on n-vertices is a simple graph in which there is no edge between any two vertices. The following null graph having 6 vertices.

2.3.9 Molecular or Chemical Graph:

A graph G is called molecular or chemical graph if vertices represents carbon atoms edges represents bonds between corresponding carbon atoms of an organic molecule.

2.4 Operations on Graphs

2.4.1 Union

Let G_1 and G_2 be two graphs then their union is defined as: $G_1 \cup G_2 = (V_1 \cup V_2, E_1 \cup E_2)$ where $V_1, E_1 \in G_1$ and $V_2, E_2 \in$

G_2.

2.4.2 Corona

Let $G_1(p_1,q_1)$, $G_2(p_2,q_2)$ be two graphs then their **Corona** of G_1 and G_2 is denoted by $G_1 \circ G_2 = G$ and is defined as: Take one copy of G_1 and p_1 copies of G_1 then join $i-th$ vertex of G_1 with $i-th$ copies of G_2

2.4.3 Sub-Graphs

Let G and H be two graphs with set of vertices and edges as $V(G)$, $E(G)$ and $V(H)$, $E(H)$, then H is said to be **sub-graph** of G if $V(H)| \subseteq |V(G)$ and $E(B)| \subseteq |E(G)$. There are different types of Subgraphs. By definition of subgraph it is not compulsory that the edge joining the two vertices must join the the vertices in Subgraph H. But whenever two of its vertices are joined by an edge in G, this edge is also in H then that Subgraph is known as *induced Subgraph*. The Particular type of Subgraph is **(Cliques)** and defined as: Set of vertices of a Graph G is known as Cliques, if each pair of vertices of Graph is joined by an edge and there is no other set which contain this set has this type of property. If Simple subgraph is induced by cliques then that Graph is a complete Graph.

2.4.4 Cyclic Graph

In cyclic graph some vertices are connected in a closed chain. If the cyclic graph contain n vertices then that graph is known as C_n. Number of vertices and edges in C_n are same and degree of each vertex is 2 i.e two edges are incident with every vertex. Following figure shows the cyclic graph.

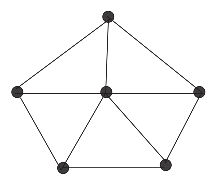

Figure 2.3: The Cyclic graph

2.4.5 Degree of a Vertex

In any Graph G, **Degree of a Vertex** is the number of edges incident to that vertex. If there is any **loop** on the vertex then the degree of that vertex will be 2. In **Regular Graphs** degree of all vertices is same as shown in the following figure. Degree of each vertex is 2. As u_1 and u_2 are the vertices of same edge then we say that u_1 and u_2 are adjacent to each other. Degree of the vertex is denoted by $d_{u_1}(G)$ or $d(u_1)$

2.4.6 Degree based topological indices

There are some Degree based topological indices as follows:

- Randic index (R_γ)
- Zagreb index (M)

- Atom-bond Connectivity index (ABC)
- Augmented Zegreb index (AZI)
- Geometric-arithmetic index (GA)
- Harmonic index (H)
- Sum-connectivity index (SCI)

Randic index

In 1975, Milan Randic introduced Randic index. Some time it is used in chemoinformatics for investigations of organic compounds. It is also called connectivity index. It is denoted by $R_{-\frac{1}{2}}$(G). The Randic index defined as:

$$R_{-\frac{1}{2}}(G) = \sum_{\alpha\beta \in E(G)} \frac{1}{\sqrt{deg(\alpha)deg(\beta)}}$$

The general Randic index $R_\gamma(G)$ is defined as:

$$R_\gamma(G) = \sum_{\alpha\beta \in E(G)} (deg(\alpha)deg(\beta))^\gamma$$

For $\gamma = -1, \;\; -\frac{1}{2}, \;\; 1, \;\; \frac{1}{2}$

M. Imran et al. extended the study of topological properties of certain networks for interconnection and drive analytical closed results of general Randic index $R_\gamma(G)$ for different values of γ for butterfly and beans network.

A. Q. Baig and M. Imran worked on different interconnection networks and derived analytical closed results of general Randic index $R_{\gamma}(G)$ for different value of γ, for dominating oxide network (DOX), dominating silicate network (DSL), triangulene oxide network (RTOX), chemical compound SiO_4

Zagreb index

I. Gutman and Trinajstic introduced Zargeb index. Balaban et al. included M_1 and M_2 among topological indices and named them Zagreb group indices. The name Zagreb group index was soon abbrev-aviated to Zagreb index, and M_1 is called the first Zagreb index and M_2 is called the second Zagreb index.

First and second Zagreb index can be defined as:

$$M_1(G) = \sum_{\alpha\beta \in E(G)} [deg(\alpha) + deg(\beta)]$$

$$M_2(G) = \sum_{\alpha\beta \in E(G)} [deg(\alpha)deg(\beta)]$$

Siddiqui et al. worked on Zegreb indices, Zagreb polynomials, first multiple Zagreb index, second multiple Zagreb index and hyper Zegren index for some nanostar dendrimers.

Atom-bond connectivity index

Estrada et al. introduced a well known connectivity index ABC, which is called Atomic-bound connectivity index. The

ABC index can be defined as:

$$ABC(G) = \sum_{\alpha\beta \in E(G)} \sqrt{\frac{d_\alpha + d_\beta - 2}{d_\alpha d_\beta}}$$

In 2010, Ghorbani et al. introduced the fourth version of ABC index, which is defined as:

$$ABC_4(G) = \sum_{\alpha\beta \in E(G)} \sqrt{\frac{S_\alpha + S_\beta - 2}{S_\alpha S_\beta}}$$

S. Hayat and M. Imran computed the fourth version of Atomic-bond connectivity index and fifth version of geometric-arithmetic index for some networks like silicate, chain silicate, hexagonal, oxide, and honeycomb networks. Atomic-bond connectivity and geometric arithmetic indices for oxide and chain silicate also computed in [**?**].

Augmented Zagreb index

By the success of the ABC index, Furtula et al. put forward its modified version, that they named augmented Zagreb index. It is defined as:

$$AZI(G) = \sum_{\alpha\beta \in E(G)} (\frac{d_\alpha(G) d_\beta(G)}{d_\alpha(G) d_\beta(G) - 2})^3$$

Geometric-arithmetic index

Geometric-arithmetic GA index which is introduced by Vukicevic et al. and defined as:

$$GA(G) = \sum_{\alpha\beta \in E(G)} \frac{2(\sqrt{d_\alpha(G) d_\beta(G)})}{(d_\alpha(G) + d_\beta(G))}$$

Fifth version of GA index GA_5 is proposed by Graovac et al. in 2011 and it defined as:

$$GA_5(G) = \sum_{\alpha\beta \in E(G)} \frac{2(\sqrt{S_\alpha(G) S_\beta(G)})}{(S_\alpha(G) + S_\beta(G))}$$

S. A. Bokhary and M. Imran worked on ABC_4 and GA_5 for certain families of dendrimers and find some formulas for them.

Nadeem et al. computed ABC_4 and GA_5 wheel, ladder and line graph of tadpole using the notion of subdivision

Harmonic index

Zhang introduced H(G) quantity, and called it harmonic index. It is defined as follows:

$$H(G) = \sum_{\alpha\beta \in E(G)} \frac{2}{d_\alpha(G) + d_\beta(G)}$$

Sum-connectivity Index

B. Zhou and N. Trinajstic introduced the sum-connectivity index. It is defined as follows:

$$SCI(G) = \sum_{\alpha\beta \in E(G)} \frac{1}{d_\alpha(G) + d_\beta(G)}$$

2.5 Distance based topological indices

The distance between the vertices of G is defined as, the distance $d(\alpha,\beta|G)$, between two vertices α and β of G is equal to the length of the shortest path connecting α and β vertices.

The history of distance based topological indices goes back to 1947, when Harold Wiener calculated the boiling points of alkanes, he used the distances in the molecular graphs of alkanes. This research of topological index is called wiener index that became most popular molecular structure descriptors.

We describe some distance based topological indices:

2.5.1 Sum of Degree of vertex

Sum of Degree of vertex is the sum of all neighboring vertices, is denoted by S_u and defined as:

$$S_u = \sum_{v \in N_G(u)} d(v)$$

where,

$$N_G(u) = v \in V(G)|uv \in E(G)$$

Let G be a finite Graph, u_1 be any vertex of G,then the Sum of degree of vertex u_1 is sum of degree of all vertices adjacent to vertex u_1. Vertices u_2 ,u_3 and u_4 are adjacent to u_1, as we know that if there is an edge between two vertices then we say that both vertices are adjacent to each other. Sum of degree of vertex u_1 is 9

2.5.2 Chemical Compounds

The Chemical Compound that contain at least one oxygen atom and one other atom in its chemical formula is known as oxide. An oxide is an ion of oxygen i.e O^{2-} where -2 is the oxidation state. The compound that contain anionic silicon compound is known as silicate. Most of the silicates are oxides. SiO_4 contain 4 oxygen ions and 1 silicon ion. These compound consist of silicate anions that is balanced by various cations and minerals are also included in it.

2.6 Graph Families

2.6.1 Complete graph

A complete graph is a simple graph in which each pair of distinct vertices are adjacent.A complete graph on n vertices is denoted by K_n, for $n \geq 3$.

2.6.2 complete bipartite

A complete bipartite graph is a graph whose vertex-set can be split into set U and V in a way that for every edge of graph G has one end point in U and another end point in V. The number of vertices of U are m and that of V,n.This graph is denoted as $B_{m,n}$.

2.6.3 regular graph

A regular graph is a graph in which all vertices have same degree. A k-regular graph is a regular graph whose common degree is k.

Chapter 3

Structural Properties of Certain Molecular Graphs

3.1 Introduction

In this chapter we will discuss the Bakelite network $(BL_{m,n})$ and find out the index of different chemical graphs. This type of structure is invented in 1907 by **Leo Hendrik Bakeland**. Bakelite was based on chemical combination of phenol and formaldehyde.

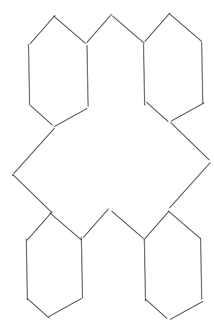

Figure 3.1: Bakelite structure

If we discuss and analize this kind of structure in graph theory such that du, dv vertices of chemical graph.

3.2 Main Discussion

According to above chemical graph there are only three types of vertices of degrees could be find that is $(2,3), (2,3), (3,3)$. There are no types of degree of vertices (du, dv) rather than of these degrees. In above chemical graph we have two rows and two coloumn . Now **m** denote the number of rows and

n represent the number of coloumn. Another type of graph is given as

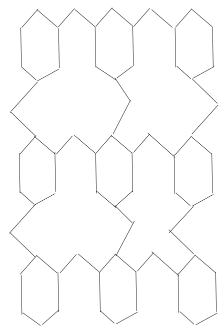

Figure 3.2: Bakelite structure

indent So this type of graph have $m = 3, n = 3$.
The table of different chemical graphs are given below.

m	n	(2,2)	(2,3)	(3,3)
2	2	10	20	2
3	3	14	56	8
4	4	18	108	18
5	5	22	176	32
6	6	26	260	50
7	7	30	360	72

In this table we elaborate the edges of different degrees of du, dv when $m = n$. Now we will discuss another type of chemical graph in which $m \neq n$ and find out the count of edges.

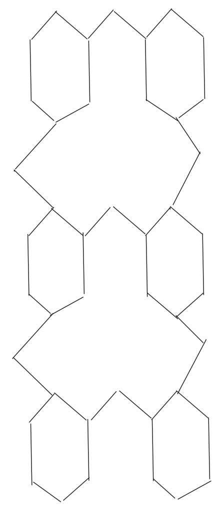

Figure 3.3: Bakelite structure for $m = 3$ and $n = 2$

In this type of graph we have $m > n$. Similarly we can draw a graph in which $n > m$.

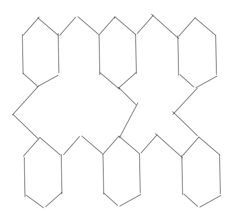

Figure 3.4: Bakelite structure for $m = 2$ and $n = 3$

Now we can draw any graph in which either $m > n$ or $n > m$ and find out the edges of degrees $(2,2),(2,3)(3,3)$. A table are given below $m > n$ and $n > m$ and count of edges of this three types of degrees.

m	n	(2,2)	(2,3)	(3,3)
2	3	12	34	4
3	2	12	34	4
3	4	16	78	12
4	3	16	78	12
4	5	20	138	24
5	4	20	138	24
5	6	24	214	40
6	5	24	214	40

3.3 Main Result

When $m \neq n$, we can see that either $m < n$ or $n < m$, it does not effect the count of edges of respective degree. In other words the count of edges will be same either $m < n$ or $m > n$. Now we want to generalized form of count of edges.
The generalized form of count of edges of degree $(2,2)$ is **2(m+n+1)** in which we putting only the values of m,n and find the count of edges directly. Similarly the degree $(2,3)$ have generalized form **[8mn-2(m+n)-4]** and for $(3,3)$ we have generalized form of count of edges is **2(m-1)(n-1)**. The more intresting thing that m,n does not depends to each other by counting of edges. We have such kind of **golden** formulas of degrees $(2,2),(2,3),(3,3)$. These golden for-

mulas will be work on all types of such kind of graphs in which either $m = n$, $m < n$, $m > n$ and $m \neq n$. We can easily find out the count of edges by simply putting the values of m, n. On the behalf of these **golden** formulas we find out the different indices such as Randic index, ABC, G(A), Hyper index and Zagreb index e.t.c Morever in this chapter we will formulated the atom bond conecctivity ABC of Bakelite network Geometric arithmatic G(A), Randic index, Zagreb index, (M_1, M_2, M_3), Hyper index, Zagreb index, Augmented Zagreb and Wiener index of Bakelite network, according to our degree based such that $(2,2), (2,3), (3,3)$ and genrelized form of count of edges of Bakelite network.

Theorem 3.3.1. *The atom bond conecctivity (ABC) of Bakelite network is*

$$ABC(BL_{m,n}) = \left(4\sqrt{2} + \frac{4}{3}\right)mn - \frac{4}{3}m - \frac{4}{3}n + \left(\frac{4}{3} - 2\sqrt{2}\right)$$

Proof

The number of vertices which have degree $(2,2)$ have $2(m+n+1)$ edges and those vertices which consist the degree $(2,3)$ have $8mn-2(m+n)-4$ edges and $(3,3)$ having count of $2(m-1)(n-1)$ edges. Since we know that,

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{du+dv-2}{dudv}}$$

This implies that

$$\begin{aligned}
ABC(BL_{m,n}) =& 2(m+n+1)\sqrt{\frac{2+2-2}{2\times 2}} + (8mn-2(m+n)-4) \\
& \sqrt{\frac{2+3-2}{2\times 3}} + 2(m-1)(n-1)\sqrt{\frac{3+3-2}{3\times 3}} \\
ABC(BL_{m,n}) =& 2(m+n+1)\frac{1}{\sqrt{2}} + (8mn-2(m+n)-4)\frac{1}{\sqrt{2}} \\
& + 2(m-1)(n-1)\frac{2}{3} \\
ABC(BL_{m,n}) =& \sqrt{2}m + \sqrt{2}n + \sqrt{2} + \frac{8mn}{\sqrt{2}} - \sqrt{2}m - \sqrt{2}n - 2\sqrt{2} \\
& + \frac{4}{3}(m-1)(n-1) \\
ABC(BL_{m,n}) =& 4\sqrt{2}mn - 2\sqrt{2} + \frac{4}{3}mn - \frac{4}{3}m - \frac{4}{3}n + \frac{4}{3}
\end{aligned}$$

Now we can write,

$$ABC(BL_{m,n}) = (4\sqrt{2}+\tfrac{4}{3})mn - \tfrac{4}{3}m - \tfrac{4}{3}n + (\tfrac{4}{3} - 2\sqrt{2}) \quad \square$$

Theorem 3.3.2. *Let the geometric arithmatic* (GA) *of Bakelite network* $(BL_{m,n})$. *Then its*$G(A)$ *index of Bakelite network is*

$$G(A)(BL_{m,n}) = (2+\frac{16\sqrt{6}}{5})mn - (\frac{4\sqrt{6}}{5})m - (\frac{4\sqrt{6}}{5})n + (4 - \frac{8\sqrt{6}}{5})$$

Proof

Since the $G(A)$ index is equal to

$$G(A) = \frac{2\sqrt{dudv}}{du+dv}$$

Therefore we can write as

$$
\begin{aligned}
G(A)(BL_{m,n}) =& 2(m+n+1)\frac{2\sqrt{2}}{2+2}+(8mn-2(m+n)-4)\frac{2\sqrt{2\times 3}}{2+3} \\
& +2(m-1)(n-1)\frac{2\sqrt{3\times 3}}{3+3} \\
G(A)(BL_{m,n}) =& 2(m+n+1)(1)+(8mn-2(m+n)-4)\frac{2\sqrt{6}}{5} \\
& +2(m-1)(n-1)(1) \\
G(A)(BL_{m,n}) =& 2(m+n+1)+(8mn-2(m+n)-4)\frac{2\sqrt{6}}{5} \\
& +2(m-1)(n-1) \\
G(A)(BL_{m,n}) =& 2m+2n+2+\frac{16\sqrt{6}}{5}mn-\frac{4\sqrt{6}}{5}m-\frac{4\sqrt{6}}{5}n-\frac{8\sqrt{6}}{5} \\
& +(2m-2)(n-1) \\
G(A)(BL_{m,n}) =& 2m+2n+2+\frac{16\sqrt{6}}{5}mn-\frac{4\sqrt{6}}{5}m-\frac{4\sqrt{6}}{5}n-\frac{8\sqrt{6}}{5} \\
& +2mn-2m-2n+2
\end{aligned}
$$

Hence we have

$G(A)(BLm,n) = (2+\frac{16\sqrt{6}}{5})mn-(\frac{4\sqrt{6}}{5})m-(\frac{4\sqrt{6}}{5})n+(4-\frac{8\sqrt{6}}{5})$ □

Theorem 3.3.3. *Let the Randic index of* $(BL_{m,n})$ *for* $a=-1$ *is defined as*

$$R_{-1}(g)=\frac{14}{9}mn+\frac{1}{18}m+\frac{1}{18}n+\frac{1}{18}$$

Proof

Since we know that

$$R_{-1}(g)=\sum_{uv\in E(G)}\frac{1}{du\times dv}$$

This implies that

$$\begin{aligned}R_{-1}(g)=&\frac{2(m+n+1)}{2\times 2}+\frac{8mn-2(m+n)-4}{2\times 3}+\frac{2(m-1)(n-1)}{3\times 3}\\=&\frac{m+n+1}{2}+\frac{4mn-m-n-2}{3}+\frac{(2m-2)(n-1)}{9}\\=&(\frac{1}{2}-\frac{1}{3}-\frac{2}{9})m+(\frac{1}{2}-\frac{1}{3}-\frac{2}{9})n+(\frac{4}{3}+\frac{2}{9})mn+(\frac{1}{2}-\frac{1}{3}-\frac{2}{9})\end{aligned}$$

Therefore,

$$R_{-1}(g)=\frac{14}{9}mn-\frac{1}{18}m-\frac{1}{18}n+\frac{1}{18}$$

$\square$

Theorem 3.3.4. *Randic index of* $(BL_{m,n})$ *then its index* $(R_{-\frac{1}{2}}(g))$ *for* $a=-\frac{1}{2}$

$$R_{-\frac{1}{2}}(G)=(4\times\sqrt{\frac{2}{3}}+\frac{2}{3})mn+(\frac{1}{3}-\sqrt{\frac{2}{3}})m+(\frac{1}{3}-\sqrt{\frac{2}{3}})n+(\frac{5}{3}-2\sqrt{\frac{2}{3}})$$

Proof

Since we know that

$$R_{\frac{-1}{2}}(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{du\times dv}}$$

This implies that

$$\begin{aligned}R_{-\frac{1}{2}}(G)=&\frac{2(m+n+1)}{\sqrt{2\times 2}}+\frac{8mn-2(m+n)-4}{\sqrt{2\times 3}}+\frac{2(m-1)(n-1)}{\sqrt{3\times 3}}\\=&m+n+1+4\sqrt{\frac{2}{3}}mn-\sqrt{\frac{2}{3}}m-\sqrt{\frac{2}{3}}n-2\sqrt{\frac{2}{3}}+\frac{2}{3}mn\\&-\frac{2}{3}m-\frac{2}{3}n+\frac{2}{3}\\R_{-\frac{1}{2}}(G)=&(4\times\sqrt{\frac{2}{3}}+\frac{2}{3})mn+(\frac{1}{3}-\sqrt{\frac{2}{3}})m+(\frac{1}{3}-\sqrt{\frac{2}{3}})n+(\frac{5}{3}-2\sqrt{\frac{2}{3}})\end{aligned}$$

$\square$

Theorem 3.3.5. *The Randic index for* $a = \frac{1}{2}$

$R_{\frac{1}{2}}(g) = (6+8\sqrt{6})mn-(2+2\sqrt{6})m-(2+2\sqrt{6})n+(10-4\sqrt{6})$

Proof

Since we know that

$$R_{\frac{1}{2}}(g) = \sum_{uv\in E(G)} \sqrt{du \times dv}$$

This implies that

$$R_{\frac{1}{2}}(g) = 2(m+n+1)\sqrt{2\times 2}+(8mn-2(m+n)-4)\sqrt{2\times 3}$$

$$+2(m-1)(n-1)(\sqrt{3\times 3})$$

$$R_{\frac{1}{2}}(g) = 4m+4n+4+8\sqrt{6}mn-2\sqrt{6}m-2\sqrt{6}n$$

$$-4\sqrt{6}+6mn-6m-6n+6$$

Hence

$R_{\frac{1}{2}}(g) = (6+8\sqrt{6})mn-(2+2\sqrt{6})m-(2+2\sqrt{6})n+(10-4\sqrt{6})$ □

Theorem 3.3.6. *The Randic index for $a = 1$*

$$R_1(g) = 2(-11m - 11n + 33mn + 1)$$

Proof

Since we also know that

$$R_1(g) = \sum_{uv \in E(G)} (du \times dv)$$

By applying the above formula we have

$$R_1(g) = 2(m+n+1)(2\times 2) + (8mn - 2(m+n) - 4)(2\times 3)$$

$$+2(m-1)(n-1)(3\times 3)$$

$R_1(g) = 8m + 8n + 8 + 48mn - 12m - 12n - 24 + 18mn - 18m - 18n + 18$
$R_1(g) = -22m - 22n + 66mn + 2$
Hence
$R_1(g) = 2(-11m - 11n + 33mn + 1)$ □

3.4 Zagreb Index

In 1972, Zagreb index has been introduced by Zagreb group Ivan Gutman and Trinajstic. We applied a family of Zagreb indices to study molecules and complexisty of selected classes of molecules. Current intrest in Zagreb indices which found use in the $QSPR|QSAR$ modeling.

Theorem 3.4.1. *The first Zagreb index of Bakelite network* $(BL_{m,n})$ *is*

$$M_1(G) = 2(26mn - 7m - 7n)$$

Proof

By using the general form of the degrees $(2,2),(2,3),(3,3)$ and count of edges with first Zagreb index. Since we know that the first Zagreb index is

$$M_1(G) = \sum_{uv \in E(G)} (du + dv)$$

This implies that
$M_1(G) = 2(m+n+1)(2+2) + [8mn - 2(m+n) - 4](2+3) + 2(m-1)(n-1)(3+3)$ $M_1(G) = 8m + 8n + 8 + 40mn - 10m - 10n - 20 = 12mn - 12m - 12n + 12$

$$M_1(G) = 52mn - 14m - 14n$$

Hence

$$M_1(G) = 2(26mn - 7m - 7n)$$

$\square$

Similarly prove that the second Zagreb index which is denoted by $M_2(G)$. And it is defined as

$$M_2(G) = \sum_{uv \in E(G)} (du \times dv)$$

Theorem 3.4.2. *The second Zagreb index of Bakelite network is equal to*

$$M_2(G) = 2(33mn - 11m - 11n + 1)$$

Proof

As we know that the second Zagreb index is defined as

$$M_2(G) = \sum_{uv \in E(G)} (du \times dv)$$

By applying this formula we have,

$$\begin{aligned} M_2(G) =& 2(m+n+1)(2\times 2) + [8mn + 2(m+n) - 4](2\times 3) \\ & + 2(m-1)(n-1)(3\times 3) \\ M_2(G) =& 8m + 8n + 8 + 48mn - 12m - 12n - 24 + 18mn \\ & - 18m - 18n + 18 \\ M_2(G) =& 66mn - 22m - 22n + 2 \end{aligned}$$

Therefore we can write as

$$M_2(G) = 2(33mn - 11m - 11n + 1)$$

$\square$

Now we discuss the third Zagreb index which is defined as given below

$$M_3(G) = \sum_{uv \in E(G)} (du - dv)$$

Theorem 3.4.3. *The third Zagreb index of Bakelite network $(BL_{m,n})$ is*

$$M_3(G) = -8mn + 2m + 2n + 4$$

Proof

Since we know that

$$M_3(G) = \sum_{uv \in E(G)} (du - dv)$$

By applying the above we have,

$$M_3(G) = 2(m+n+1)(2-2) + [8mn - 2(m+n) - 4](2-3) + 2(m-1)(n-1)(3-3)$$

$$M_3(G) = -8mn + 2m + 2n + 4$$

□

3.5 Hyper Zagreb Index

The Hyper Zagreb index is denoted by HMG. And it is defined as

$$HM(G) = \sum_{uv \in E(G)} (du + dv)^2$$

Where du denote the first vertex and dv denote the second vertex of graph G.

Theorem 3.5.1. *Let the Hyper Zagreb index of Bakelite network* ($BL_{m,n}$ *is*

$$HMG = -90m - 90n + 207mn + 4$$

Proof

Since also know that

$$HM(G) = \sum_{uv \in E(G)} (du + dv)^2$$

now by applying this we have

$$HM(G) = 2(m+n+1)(2+2)^2 + [8mn - 2(m+n) - 4](2+3)^2$$

$$+2(m+n)(n-1)(3+3)^2$$

$$HM(G) = 32m + 32n + 32 + 200mn - 50m - 50n - 100 + 72mn$$

$$-72m - 72n + 72$$

Hence after rearranging we have

$$HM(G) = 272mn - 90m - 90n + 4$$

$\square$

3.6 Harmonic Index

Zhang itroduced $H(G)$ quantity and called it harmonic index. It is defined as fallow.

$$H(G) = \sum_{uv \in E(G)} \frac{2}{du + dv}$$

Theorem 3.6.1. *Let G be the graph of harmonic index of Bakelite network $BL_{m,n}$. The Harmonic index of Bakelite structure $(BL_{m,n})$ is equal to*

$$H(G)(BL_{m,n}) = \frac{58}{15}mn - \frac{7}{15}m - \frac{7}{15}n + \frac{1}{15}$$

Proof

The harmonic index of Bakelite network is defined as given as

$$H(G)(BL_{m,n}) = \sum_{uv \in E(G)} \frac{2}{du + dv}$$

by appling above formula we have for degrees $(2,2),(2,3),(3,3)$ the harmonic index

$$
\begin{aligned}
Ha(G)(BL_{m,n}) =& \frac{2(m+n+1)2}{2+3} \\
&+ \frac{2\times(m-1)(n-1)\times 2}{3+3} \\
H(G)(BL_{m,n}) =& m+n+1+\frac{2}{5}(8mn-2m-2n-4)+\frac{2}{3}(m-1)(n-1) \\
H(G)(BL_{m,n}) =& m+n++1+\frac{16}{5}mn-\frac{4}{5}m-\frac{4}{5}n-\frac{8}{5}+\frac{2}{3}mn \\
&-\frac{2}{3}m-\frac{2}{3}n+\frac{2}{3}
\end{aligned}
$$

After rearranging we have

$$
H(G)(BL_{m,n}) = \frac{58}{15}mn - \frac{7}{15}m - \frac{7}{15}n + \frac{1}{15}
$$

$\square$

3.7 Augmented Zagreb Index

By the success of the ABC index. Further et.al. put forward its modified version, that they named Augmented Zagreb index. Its defined as

$$AZI(G) = \sum_{uv \in E(G)} (\frac{dudv}{dudv - 2})^3$$

Theorem 3.7.1. *Let the Augmented Zagreb index of Bakelite* $(BL_{m,n})$ *is equal to as*

$$AZI(G) = \frac{10719}{343}mn + \frac{6859}{1372}m + \frac{6859}{1372}n + \frac{4631}{686}$$

Proof

According to our degree based topological indices od degrees $(2,2),(2,3),(3,3)$ and count of edges $2(m+n+1), 8mn-2(m+n)-4and2(m-1)(n-1)$. now by appling the formula of AZI we he have

$$AZI(G) = 2(m+n+1)(\frac{2\times 2}{2\times 2-2})^3 + (8mn-(m+n)-4)(\frac{2\times 3}{2\times 3-2})^3$$

$$+2(m-1)(n-1)(\frac{3\times 3}{3\times 3-2})^3$$

$$AZI(G) = 16m + 16n + 16 + 27mn - \frac{27}{4}m - \frac{27}{4}n - \frac{27}{2} + \frac{1458}{343}mn$$

$$-\frac{1458}{343}m-\frac{1458}{343}n+\frac{1458}{343}$$

After arranging the coefficient of mn,m,n and constant we have

$$AZI(G)=\frac{10719}{343}mn+\frac{6859}{1372}m+\frac{6859}{1372}n+\frac{4631}{686}$$

$\square$

Chapter 4

Conclusion and Closing Remarks

In this paper, certain degree based topological indices, namely general Randic index, Atomic-bond conecctivity index (ABC), geometric, Arithmatic index G(A), Zagreb index such as Hyper Zagreb index, Augmented Zagreb index, first, second and third Zagreb index for Bakelite network $(BL_{m,n})$ were studied for the first time. To construct and study new architectures has always been an open problems in both network and art design sciences.

In further, we interested to design some new architectures networks and then study their topological indices which will be quite helpful to understand their underlying topologies. By calculating the several topological indices for these molecules and performing some kind of statistical analysis a correlation between experimental values and values of topological indices can be found...

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