# THE FIRST AND SECOND ZAGREB INDICES TO MOLECULAR GRAPHS OF ALKANES, $C_nH_{(2n+2)}$

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## Abstract.

*For a simple graph $G = (V(G), E(G))$, let $d(u)$, $d(v)$ be the degree of the vertices $u$, and $v$ in $G$. The first and second Zagreb indices of G are defined as*
$M_1(G) = \sum_{e=uv\in E(G)}(d(u)+d(v))$ *and* $M_2(G) = \sum_{e=uu\in E(G)} d(u)d(v)$, *respectively.*
*The first, generalized, and the second Multiplicative Zagreb indices of simple graph G are defined as*
$PM_1(G) = \prod_{e=uv\in E(G)}(d(u)+d(v))$ *and* $PM_2(G) = \prod_{e=uu\in E(G)}(d(u)d(v))$
*respectively. The multiplicative Zagreb indices have been the focus of considerable research in computational chemistry dating back to Narumi and Katayama in 1980s.*

*The general class of molecules known as the alkanes, or paraffins, is given by chemical formula* $\boldsymbol{C_nH_{(2n+2)}}$ *and it is natural to ask how many different molecules, number of atoms are there a with this formula. We derive a simple formula to find the first and second Zagreb indices for any positive integer $n$, show formulate a python approach to find a vertex distance matrix from a vertex incidence matrix, formulate Zagreb indices by $(d(e))$, the degree set of adjacent edges, and prove*
$M_1(G) = \sum_{e\in E(G)} d(e) + \sum_{u\in V(G)} d(u)$,
$\sum_{e=uv\in E(G)}(d(u))^2 + (d(v))^2 = \sum_{u\in V(G)}(d(u))^3$
*and the First and the second multiplicative Zagreb indices of a graph G*
$PM_1(G) = \prod_{e=uv\in E(G)}(d(e)+2)$ *and* $PM_2(G) = \prod_{u\in V(G)}(d(u))^{(d(u))}$

**Keywords:** *Zagreb index · Multiplicative Zagreb index · Alkanes.*

**INTRODUCTION**

A graph is a collection of points together with a number of lines connecting a subset of them. The points and lines of a graph are called vertices and edges of the graph, respectively. The vertex and edge sets of a graph G are denoted by V (G) and $E(G)$, or briefly by $V$ and $E$, respectively. If we think of molecules as particular chemical structures, and if we replace atoms and bonds with vertices and edges, respectively, the obtained graph is called a molecular graph. That is, a molecular graph is a simple graph such that its vertices correspond to the atoms and its edges to the bonds. Note that hydrogen atoms are often omitted and the remaining part of the graph is sometimes called as the carbon graph of the corresponding molecule. Chemical graph theory which deals with the above-mentioned relations between molecules and corresponding graphs is a branch of mathematical chemistry which has an important effect on the development of the molecular chemistry.

A topological graph index is a numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity.

As an example, the boiling point of a molecule is directly related to the forces between the atoms. When a solution is heated, the temperature is increased and as it is increased, the kinetic energy between molecules increases. This means that the molecular motion becomes so intense that the bonds between molecules break and become a gas. The moment the liquid turns to gas is labeled as the boiling point. The boiling point can give important clues about the physical properties of chemical structures. Molecules which strongly interact or bond with each other through a variety of intermolecular forces cannot move easily or rapidly and therefore, do not achieve the kinetic energy necessary to escape the liquid state. That is why the boiling points of the alkanes increase with molecular size. Two of the most useful topological graph indices are the first and second Zagreb indices which have been introduced by Gutman and Trinajstic in [6].

Chemical graph theory is a branch of mathematics which combines graph theory and chemistry. Graph theory is used to mathematically model molecules in order to gain insight into the physical properties of these chemical compounds. Some physical properties, such as the boiling point, are related to the geometric structure of the compound. This is especially true in the case of chemical compounds as an alkane. Alkanes are organic compounds exclusively composed of carbons and hydrogen atoms.

In this paper molecular graph referred as a simple finite undirected and connected graph. In chemical graph theory, the molecular structure of a compound is often presented with a graph, where the atoms of the chemical compound are represented by vertices and edges represent the chemical bonds.

Let G= (V, E) is a graph with vertex set V = $\{v_1, v_2, v_3, - - -, v_{n-1}, v_n\}$ and the edge set
E = $\{e_1, e_2, e_3, - - -, e_{n-2}, e_{n-1}\}$ where $e_i = v_i v_{i+1}$ for each I, $1 \leq i \leq n-1$. Two vertices are called adjacent if there is an edge that connects them. In this case vertices are called end points of the edge and vertices are incident to the edge.

**Definition I:** The set of all vertices adjacent to a specific vertex v is called the open neighbored of v and denoted by $N_G(v)$ or $N(v)$.
**Definition II:** The number of edges that a vertex $v$ is incident to in a graph $G = (V, E)$ is called the degree of the vertex v and is denoted $deg(v)$. Note: deg(v) = | $N_G(v)$| or |$N(v)$|.

A $u - v$ path in a graph $G$ is a sequence of distinct vertices $uv_1$, $v_1v_2$, $v_2v_3$ , . . ., $v_nv$ in $G$ such that each vertex is adjacent to the next. The length of $u$-$v$ path is the number of edges on this path.

**Definition III**: The distance between two vertices $u, v \in V(G)$ denoted by $d(u, v)$ is the number of edges on the shortest path between them in G.

Degree sequence of a graph is the list of degree of all the vertices of the graph. Usually, we list the degree in nonincreasing order, that is from largest to the smallest.
D = $(d_1, d_2, d_{3,}, - - -, d_{n-1}, d_n)$ is a degree sequence of a graph G with |V| = $n$ such that $d_i = \deg(v_i)$.

**Handshaking Theorem I:** The sum of degrees of the vertices of a graph G = (V , E) is twice the number of vertices. That is

$$\sum_{i=1}^{n} \deg(v_i) = \sum_{i=1}^{n} (d_i) = 2|E|$$

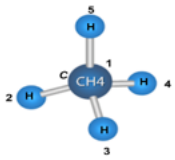
where $|E|$ represent the number of edges of the graph G = (V , E)

**Vertex Adjacency matrix:** The Vertex Adjacency matrix, also called the connection matrix, is a matrix containing rows and columns which is used to represent a simple labelled graph, with 0 and 1in the position of $(v_i, v_j)$ according to the condition whether $v_i$ and $v_j$ are adjacent or not.
Note: Adjacency matrix is a symmetric matrix of size n by n, where $|V| = n$.

$$\text{VAM} = (v_{ij}) = \begin{cases} 1 \ ; \text{ if } v_i \text{ and } v_j \text{ are adjacent} \\ 0 \ ; \quad \text{otherwise} \end{cases}$$

**Vertex Distance Matrix:** Also called the standard distance matrix of a vertex labelled connected graph is a symmetric $n$ by $n$ matrix where $n = |V|$ whose elements are defined as:

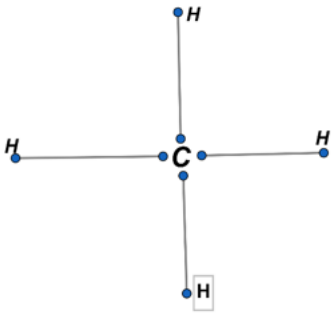
$$\text{VDM} = (d_{ij}) = \begin{cases} d(i,j) \ ; \text{ if } i \neq j \\ 0 \ ; \quad \text{otherwise} \end{cases}$$




**Example I**

Given a graph G = (V, E) = $C_1H_4 = CH_4$

$$\text{VAM} = (v_{ij}) = \begin{pmatrix} * & 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 2 & 1 & 0 & 0 & 0 & 0 \\ 3 & 1 & 0 & 0 & 0 & 0 \\ 4 & 1 & 0 & 0 & 0 & 0 \\ 5 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$




$$\text{VDM} = (v_{ij}) = \begin{pmatrix} * & 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 2 & 1 & 0 & 2 & 2 & 2 \\ 3 & 1 & 2 & 0 & 2 & 2 \\ 4 & 1 & 2 & 2 & 0 & 2 \\ 5 & 1 & 2 & 2 & 2 & 0 \end{pmatrix}$$

Among the oldest and most student topological indices, there are two classical vertex-degree based topological indices, the first Zagreb index and second Zagreb index. These two indices first introduced more than thirty years ago by Gutman and Trinajstic' in [14], and were explained in [15]. Later they were used in the structure property model {20]. The first and Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a graph G are defined, respectively, as

The First Zagreb index = $M_1(G) = \sum_{u \in V(G)} (d(u))^2$

and

The second Zagreb Index = $M_2(G) = \sum_{e=uu \in E(G)} d(u)d(v)$

During the past years, numerous results concerning Zagreb indices have been put forward, the first and second multiplicative indices [11.18.19] are defined as follows

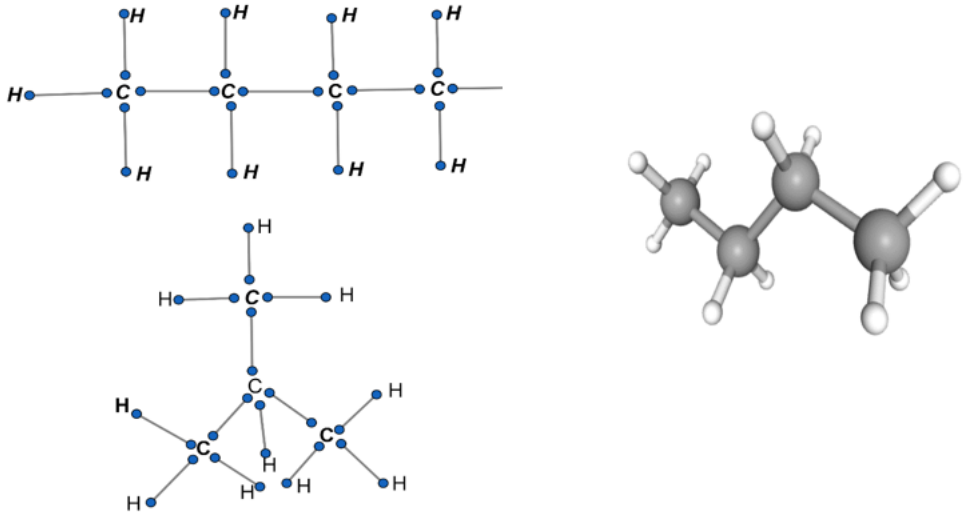
$$\prod_1 (G) = \prod_{u \in V(G)} (d(u))^2$$

and

$$\prod_2 (G) = \prod_{e=un \in E(G)} (d(u)d(v)) = \prod (d(u))^{d(u)}$$

Details on the chemical applications of the two Zagreb indices can be found in the books [12, 13]. Further studies on Zagreb indices can be found in [1, 6, 16, 17, 18].

**Enumeration of chemical molecules**: One of the earlies uses of trees was in the enumeration of Chemical molecules. If we have a molecule consisting only of carbon atoms and hydrogen atoms, then we can represent it as a graph in which each carbon appears as a vertex of degree 4, and each hydrogen atom appears as a vertex of degree 1. The graph of n-butane and 2-methyl propane are shown in the figure below. Although they have the same chemical formula $C_4H_{10}$ , they are different molecules because the atoms are arranged differently within the molecules. These two molecules form part of a general class of molecules known as the alkanes, or paraffins, with chemical formula $C_nH_{(2n+2)}$, and it is natural to ask how many different molecules there are with this formula.



**Theorem II:** The graph $G = (V, E)$ of any molecule with the formula $C_nH_{(2n+2)}$ has order $|V| = (3n + 2)$ and size $|E| = (3n + 1)$ edges.

**Proof:**
Number of vertices of a graph G is the sum of number of Hydrogens and Carbon atoms. That is $|V| = n + (2n + 2) = 3n + 2$. There are $(2n + 2)$ edges between each hydrogen atom and a carbon atom. There is an edge between two carbon atoms which implies the total number of edges between carbon atoms is $(n - 1)$. Any two-hydrogen atom is not adjacent. Therefore,
$|E| = (2n + 2) + (n - 1) = (3n + 1)$.

***Definition IV:*** The **lexicographic order** on words is the relation defined by $X < Y$ comes strictly before $Y$ in the dictionary order. Here's a more formal definition. First, we order the alphabet in the obvious way $\boldsymbol{a < b < c < d < - - - < w < x < y < z}$ **.**
***Choose a Row that has 1***. Move from the value 1 row down to the column. If there are more than 1's in this column, we have that numbers of distance 2.
After moving a row down to a column, then move to the left in the same row to find 1. If you see 1 down this column you have distances 3. Otherwise, stop there.
**Choose another row** that has 1. Move to the left and find 1. If you did not find 1, then distance is 1. If you see 1, then that is continue the process till you find the maximum \ distance. Keep the process. Since the matrix is symmetric, we can perform the operation either the upper or the lower half of the principal diagonal.

***Theorem III:*** We can find the vertex distance matrix from the vertex adjacency matrix using lexicographic order. The words are Rows.

***Example:***
***Consider the graph above with vertex adjacency matrix.***

$$\mathbf{VAM} = (v_{ij}) = \begin{pmatrix} * & 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 2 & 1 & 0 & 0 & 0 & 0 \\ 3 & 1 & 0 & 0 & 0 & 0 \\ 4 & 1 & 0 & 0 & 0 & 0 \\ 5 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} * & 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 2 & 1 & 0 & 0 & 0 & 0 \\ 3 & 1 & 0 & 0 & 0 & 0 \\ 4 & 1 & 0 & 0 & 0 & 0 \\ 5 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} * & 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 2 & 1 & 0 & 0 & 0 & 0 \\ 3 & 1 & 0 & 0 & 0 & 0 \\ 4 & 1 & 0 & 0 & 0 & 0 \\ 5 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

- $\mathbf{1 \to 2}$ $\mathbf{1 \to 3}$ $\mathbf{1 \to 4}$ $\mathbf{1 \to 5}$
  $\mathbf{d(1,2) = d(1,3) = d(1,4) = d(1,5) = 1}$
- $\mathbf{2 \to 1 \to 3}$ $\mathbf{2 \to 1 \to 4}$ ***and*** $\mathbf{2 \to 1 \to 5}$
  $\mathbf{d(2,3) = d(2,4) = d(2,5) = 2}$
- $\mathbf{3 \to 1 \to 4}$ $\mathbf{3 \to 1 \to 5}$ ***and*** $\mathbf{3 \to 1 \to 2}$
  $\mathbf{d(3,4) = d(3,5) = d(3,2) = 2}$

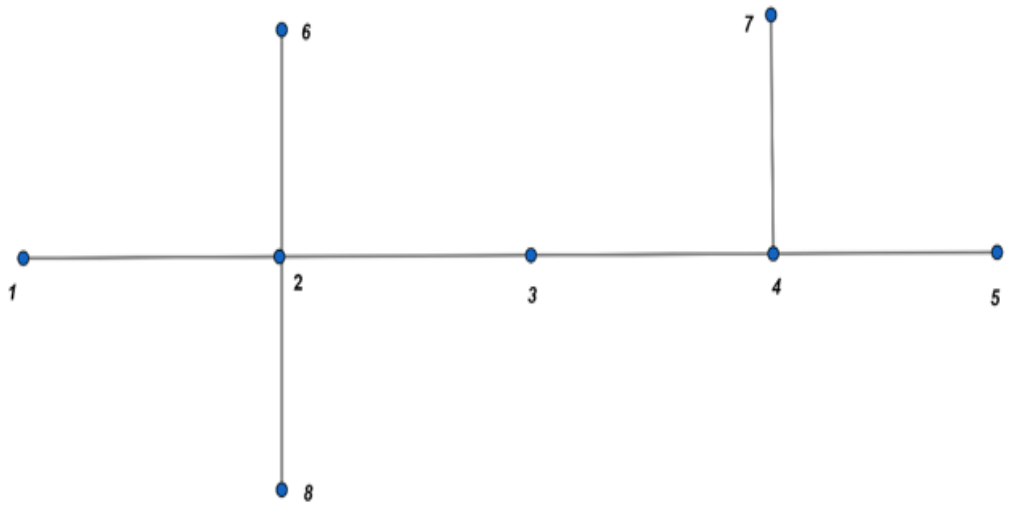
$$\mathbf{VAM} = (v_{ij}) = \begin{pmatrix} * & 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 2 & 1 & 0 & 0 & 0 & 0 \\ 3 & 1 & 0 & 0 & 0 & 0 \\ 4 & 1 & 0 & 0 & 0 & 0 \\ 5 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} * & 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 2 & 1 & 0 & 0 & 0 & 0 \\ 3 & 1 & 0 & 0 & 0 & 0 \\ 4 & 1 & 0 & 0 & 0 & 0 \\ 5 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} * & 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 2 & 1 & 0 & 0 & 0 & 0 \\ 3 & 1 & 0 & 0 & 0 & 0 \\ 4 & 1 & 0 & 0 & 0 & 0 \\ 5 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$\mathbf{d(3,4) = 2}$ $\mathbf{d(3,5) = 2}$ $\mathbf{d(3,2) = 2}$

Hence:

$$\mathbf{VDM} = (v_{ij}) = \begin{pmatrix} * & 1 & 2 & 3 & 4 & 5 \\ 1 & d(1,1) & d(1,2) & d(1,3) & d(1,4) & d(1,5) \\ 2 & d(2,1) & d(2,2) & d(2,3) & d(2,4) & d(2,5) \\ 3 & d(3,1) & d(3,2) & d(3,3) & d(3,4) & d(3,5) \\ 4 & d(4,1) & d(4,2) & d(4,3) & d(4,4) & d(4,5) \\ 5 & d(5,1) & d(5,2) & d(5,3) & d(5,4) & d(5,5) \end{pmatrix}$$

**Example 2:**



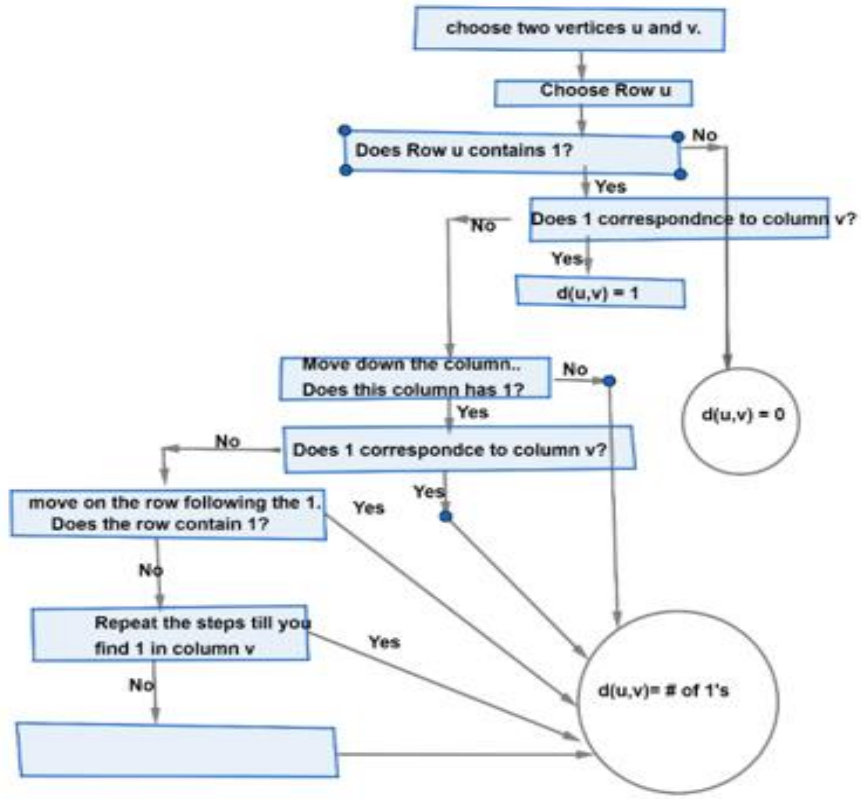

The graph represents 2,2,4 – trimethylpentane with the hydrogen atoms removed called a carbon tree. Hydrogen depleted Molecular graph.

$$\mathbf{VAM} = (v_{ij}) = \begin{pmatrix} * & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 3 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 5 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 6 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 7 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 8 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \mathbf{VAM} = (v_{ij}) = \begin{pmatrix} * & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 3 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 5 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 6 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 7 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 8 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

A) $1 \rightarrow 2$ $d(1,2) = 1$ C) $1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 5$ $d(1,5) = 4$
B) $1 \rightarrow 2 \rightarrow 3$ *and* $1 \rightarrow 2 \rightarrow 6$ *and* $1 \rightarrow 2 \rightarrow 8$ $d(1,3) = d(1,6) = d(1,8) = 2$
D) $1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 7$ $d(1,7) = 4$

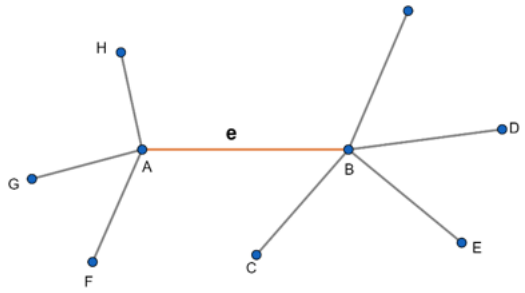
$$\mathbf{VAM} = (v_{ij}) = \begin{pmatrix} * & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 3 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 5 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 6 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 7 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 8 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad \mathbf{VAM} = (v_{ij}) = \begin{pmatrix} * & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 3 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 5 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 6 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 7 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 8 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

A) $8 \rightarrow 2 \rightarrow 6$ d (8, 6) = 2 C) $\mathbf{8 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 5}$ d (8,5) = 4
B) $1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 5$ d (1, 5) = 4




**Theorem IV**: In a simple $G = (V, E)$ that represents the $C_nH_{(2n+2)}$, for e = AB ∈ E(G) , the degree of $e$ , $d(e) = d(A) + d(B) - 2$.

**Proof.** The degree of edge $e = AB$ equals the number of edges incident from both vertices




$A$ *and* $B$. This equals the sum of the degree of the two vertices minus two because we count the end points of $e$ twice as the degree sum.
deg(A) = 4 and deg(B) = 5 but deg (e) = 3 + 3 = 6 = deg ( A) + deg( B) − 2

**Theorem V** For the simple graph $G = (V, E)$ , and the edge set E(G) = {e: e = uv, where u , v ∈ V(G)}
$\sum_{e=uv\in E(G)}(d(u))^2 + (d(v))^2 = \sum_{a\in V(G)}(d(a))^3$

**Proof:**
For each edge $e = uv$, $d(u)$ and $d(v)$ are multiplied with $d(u)$ and $d(v)$ number of different vertices respectively. Because there are $d(u)$ and $d(v)$ number of edges incident to each.

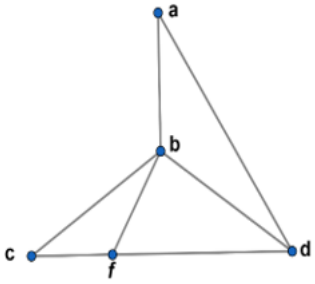
This implies, $u$ is adjacent to vertices say $u_1, u_2, u_3, - - -, u_{d(u)}$, and we count
$(d(u))^2 + (d(u_i))^2$ for each $i = 1, 2, 3, - - -, d(u)$

This implies we have for each $u$ and $v$ such that $e = uv$ , $(d(u))^2$ and $(d(v))^2$ can be counted $d(u)$ and $d(v)$ times each respectively.

Hence, we have
$d(u)^* (d(u))^2 = (d(u))^3$ for each end vertices and results
$\sum_{e=uv\in E(G)}(d(u))^2 + (d(v))^2 = \sum_{a\in V(G)}(d(a))^3$ .

**Example III**

*Consider the graph G = (V, E)*




The edge set E(G) = {*ab, bc, bd, bf, ad, cf, fd*}

**Definition V:** The hyper Zagreb index of simple connected graph G = (V, E) was introduced by G.H Shirdel, H Rezapour and, A M Sayadi. It is defined as [11]

| **edge** | **degree** | | | | $(\deg(u))^2+(\deg(v))^2$ | $(\deg(u))^3$ |
|---|---|---|---|---|---|---|
| *ab* | *deg(a)* | **2** | deg(b) | **4** | $2^2+4^2=20$ | $(\deg(a))^3=(2)^3=8$ |
| *bc* | *deg(b)* | **4** | deg(c) | **2** | $4^2+2^2=20$ | $(\deg(b))^3=(4)^3=64$ |
| *bd* | *deg(b)* | **4** | deg(d) | **3** | $4^2+3^2=25$ | $(\deg(c))^3=(3)^3=27$ |
| *ad* | *deg(a)* | **2** | deg(d) | **3** | $2^2+3^2=13$ | $(\deg(d))^3=(3)^3=27$ |
| *cf* | *deg(c)* | **2** | deg(f) | **3** | $2^2+3^2=13$ | $(\deg(f))^3=(2)^3=8$ |
| *fd* | *deg(f)* | **3** | deg(d) | **3** | $3^2+3^2=18$ | |
| *bf* | *deg(b)* | **4** | deg(f) | **3** | $4^2+3^2=25$ | |
| | | | | | $\sum_{f=uv\in E(G)}((\deg(u))^2+(\deg(v))^2)=134$ | $\sum_{u\in V(G)}(\deg(u))^3=134$ |

*Hyper Zagreb Index of G =* $M_H(G)=\sum_{e=uv\in E(G)}(deg(u)+deg(v))^2$

**Theorem VI**

The hyper Zagreb Index of G = $M_H(G)=\sum_{u\in V(G)}(d(u))^3+2M_2(G)$

**Proof:**

$$M_H(G)=\sum_{e=uv\in E(G)}(deg(u)+deg(v))^2=\sum_{e=uv\in E(G)}((d(u))^2+2d(u)d(v)+(d(v))^2)$$

$$=\sum_{e=uv\in E(G)}\left((d(u))^2+(d(v))^2\right)+\sum_{e=uv\in E(G)}2*d(u)d(v)$$

$$=\sum_{u\in V(G)}(d(u))^3+2*\sum_{e=uv\in E(G)}d(u)d(v)$$

$$=\sum_{u\in V(G)}(d(u))^3+2*M_2(G)$$

**Theorem VII**

Hyper Zagreb Indices HZI of G = $M_H(G)=\sum_{e\in E(G)}(d(e)+2)^2$.

*Proof:*

$d(u)+d(v)=d(e)+2$ *where* $e=uv\in E(G)$. *This implies*

$(d(u)+d(v))^2=(d(e)+2)^2$ *and then* $\sum_{e=uv\in E(G)}(deg(u)+deg(v))^2$

$=\sum_{e=uv\in E(G)}(deg(e)+2)^2$.

*Hence* $M_H(G)=\sum_{e\in E(G)}(d(e)+2)^2$.

***Theorem VIII***

$M_H(G)=\sum_{u\in V(G)}(d(u))^3+2*M_2(G)$

***Proof:***

$M_H(G)=\sum_{e\in E(G)}(d(u)+d(v))^2$

$=\sum_{e\in E(G)}(deg(e)+2)^2$ because, $deg(e)=d(u)+d(v)-2$

*which* imply $deg(e)+2=d(u)+d(v)$

$$=\sum_{u\in V(G)}(d(u)+\deg(v))^2$$

$$=\sum_{e=uv\in E(G)}\left((d(u))^2+(d(v))^2\right)+\sum_{e=uv\in E(G)}d(u)d(v)$$

$$=\sum_{u\in V(G)}(d(u))^3+2\sum_{e=uv\in E(G)}d(u)d(v)$$

$$=\sum_{u\in V(G)}(d(u))^3+2*M_2(G)$$

**Theorem IX**
The first Zagreb index $M_1(G) = \sum_{e \in E(G)} d(e) + \sum_{u \in V(G)} d(u)$.

**Proof:**
$\sum_{e \in E(G)} d(e) = \sum_{e=uv \in E(G)} (d(u) + d(v) - 2)$ *for* $d(e) = d(u) + d(v) - 2$
$= \sum_{e=uv \in E(G)} \big(d(u) + d(v)\big) - \sum_{e=uv \in E(G)} 2$
$= M_1(G) - \sum_{e=uv \in E(G)} (2)$
$= M_1(G) - \sum_{e=uv \in E(G)} (2) = M_1(G) - \sum_{u \in V(G)} d(v)$ *Handshaking Lemma*

*Hence*
$$M_1(G) = \sum_{e \in E(G)} d(e) + \sum_{u \in V(G)} d(v)$$

***Theorem X***
The second Zagreb index c
$M_2(G) = \frac{1}{2} * \left(\sum_{e \in E(G)} (d(e) + 2)^2 - \sum_{u \in V(G)} (d(u))^3\right)$.

**Proof:**
$\sum_{e=uv \in E(G)} (d(u) + d(v))^2 = \sum_{e \in E(G)} \left(\big(d(u)\big)^2 + \big(d(v)\big)^2 + 2d(u)d(v)\right)$
$= \sum_{e \in E(G)} \left(\big(d(u)\big)^2 + \big(d(v)\big)^2\right) + \sum_{e \in E(G)} (2d(u)d(v))$
$= \sum_{e \in E(G)} \left(\big(d(u)\big)^3\right) + 2*M_2(G)$

This implies,
$$\sum_{e \in E(G)} (d(e) + 2)^2 = \sum_{u \in V(G)} \left(\big(d(u)\big)^3\right) + 2*M_2(G)$$
and then,
$$2*M_2(G) = \sum_{e \in E(G)} (d(e) + 2)^2 - \sum_{e \in E(G)} \left(\big(d(u)\big)^3\right)$$

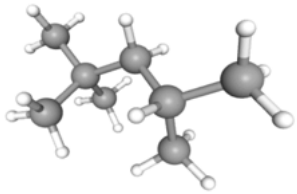
Hence:
$$M_2(G) = \frac{1}{2} * \left(\sum_{e \in E(G)} (d(e) + 2)^2 - \sum_{u \in V(G)} \left(\big(d(u)\big)^3\right)\right)$$

**Theorem XI**
Given the graph of $G = (V, E) = C_n H_{(2n+2)}$. The first Zagreb index $M_1(G)$ is give by
I) $M_1(G) = 18n + 2$ and
II) $M_2(G) = 24n - 8$

**Proof:**
I) $M_1(G) = \left(\sum_{e=uv \in E(G)} d(u) + d(v)\right) = \sum_{e \in E(G)} d(e) + \sum_{u \in V(G)} d(v)$
$= \sum_{i=1}^{2n+2} d_e(H_i) + \sum_{i=1}^{n-1} d_e(C_i) + \sum_{i=1}^{2n+2} d(H_i) + \sum_{i=1}^{n} d(C_i)$
$= 3(2n + 2) + 6(n - 1) + (2n + 2) + 4(n)$
$= 6n + 6 + 6n - 6 + 6n + 2$
$= 18n + 2$

II) $M_2(G) = \frac{1}{2} * \left(\sum_{e \in E(G)} (d(e) + 2)^2 - \sum_{u \in V(G)} \left(\big(d(u)\big)^3\right)\right)$
$= \frac{1}{2} * \left(\sum_{i=1}^{2n+2} (d_e(H_i) + 2)^2 + \sum_{i=1}^{n-1} (d_e(C_i) + 2)^2\right) - \frac{1}{2} * \sum_{H_i \in V(G)} \left(\big(d(H_i)\big)^3\right)$
$- \frac{1}{2} * \sum_{C_i \in V(G)} \left(\big(d(C_i)\big)^3\right)$
$= \frac{1}{2} * \left(\sum_{i=1}^{2n+2} (3 + 2)^2 + \sum_{i=1}^{n-1} (8)^2\right) - \frac{1}{2} * \sum_{i=1}^{2n+2} (1)^3$
$- \frac{1}{2} * \sum_{i=1}^{n} ((4)^3)$
$= \frac{1}{2} * (25(2n + 2) + 64(n - 1) - (2n + 2) - 64(n))$
$= \frac{1}{2} * (50n + 50 + 64n - 64 - 2n - 2 - 64n)$
$= \frac{1}{2} * (48n - 16)$
$= 24n - 8$

***Example IV***
Calculate the first and second Zagreb indices for chemical graph 2,2,4-trimetylpentane molecule.



Answer: Chemical formula is $G(V, E) = C_8H_{18} = C_nH_{(2n+2)}$ .

$M_1(G) = 18(n) + 2 = 18(8) + 2$

$= 16(8) + 2(8) + 2 = 8 * (4^2) + 18(1)$

$= \left(\sum_{u \in V(G)} (d(u))^2\right) = 146.$

$M_2(G) = 24 * (n) - 2 = 24 * (8) - 8 =$

$= 18 * (1 * 4) + (4 * (4)) * 7$

$= \sum_{e=uu \in E(G)} d(u)d(v) = 184.$

In 2012, Ghorbani and Azimi [6] proposed the multiplicative versions of Zagreb indices of a graph G. These new indices are first multiple Zagreb index $PM_1(G)$ and second multiple Zagreb index $PM_2(G)$ and are defined as

$PM_1(G) = \prod_{e=uv \in E(G)} (d(u) + d(v))$ **and** $PM_2(G) = \prod_{e=uv \in E(G)} (d(u)d(v))$

**Theorem XII**

The First and the second multiplicative Zagreb indices of a graph G that represent the chemical formula $\mathbf{C_nH_{(2n+2)}}$ are respectively

I) $PM_1(G) = \left(\frac{25}{8}\right) * (200)^{(n)}$ and II) $PM_2(G) = (16)^n$

**Proof:**

I) $PM_1(G) = \prod_{e=uv \in E(G)} (d(u) + d(v))$

There are $n$ carbons and $(2n + 2)$ hydrogen atoms. Each hydrogen atom is incident to exactly one carbon atom where $d(H_i) = 1$ for each $i$ where $1 \leq i \leq (2n + 2)$, and the number of edges incident to a carbon - carbon atoms are $(n - 1)$ where $d(C_i) = 4$.

This implies

$PM_1(G) = \prod_{e=uv \in E(G)} (d(u) + d(v)) = \prod_{e=uv \in E(G)} (d(H_i) + d(C_i)) * \prod_{e=uv \in E(G)} (d(C_i) + d(C_j))$

$= \prod_{i=1}^{(2n+2)} (1 + 4) * \prod_{i=1}^{(n-1)} (4 + 4)$ ( where the first product shows the edge between $H_i$ and $C_i$ and the second product between two adjacent carbon atoms.)

$= 5^{(2n+2)} * 8^{(n-1)} = 5^{(n-1)} * 5^{(n-1)} 5^{(4)} * 8^{(n-1)}$

$= (625) * (200)^{(n-1)}$

$= \left(\frac{25}{8}\right) * (200)^{(n)}$

II)

$PM_2(G) = \prod_{e=uv \in E(G)} (d(u)d(v)) =$

$= \prod_{e=uv \in E(G)} (d(H_i) * d(C_i)) * \prod_{e=uv \in E(G)} (d(C_i) * d(C_j))$

$= \prod_{i=1}^{(2n+2)} (d(H_i) * d(C_i)) * \prod_{i=1}^{(n-1)} (d(c_i) * d(C_i))$

$= \prod_{i=1}^{(2n+2)} (1 * 4) * \prod_{i=1}^{(n-1)} (4 * 4)$

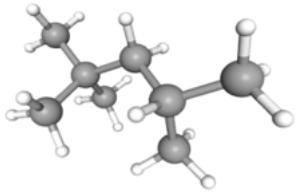
$= (4)^{(2n+2)} * (16)^{(n-1)}$

$= (4)^{(2n+2)} * (4)^{(2n-2)}$

$= (4)^{(4n)}$

$= (16)^n$

**Example V:** consider a chemical graph for 2,2,4-Trimethylpentane, $\mathbf{C_8H_{(18)}}$



Calculate the First and the Second multiplicative Zagreb indices of a graph G = $C_8H_{(18)}$

Answers:
Given n = 8 .

I) $PM_1(G) = \prod_{e=uv\in E(G)}(d(u)+d(v))$ =

$= (1+4)*(1+4)*---(1+4)*(4+4)*(4+4)*---(4*4)$

$(2n+2)$ times $(n-1)$ times

$= (5 * 5 * 5 * --- *5)\ \&\ (8* 8* 8* --- *8)$

$= (5)^{(18)} * (8)^{(7)} = (25)^{(9)} * (8)^{(7)}$

$= \left(\frac{25}{8}\right) * (200)^{(n)} = 625* (200)^{(n-1)}$

II) $PM_2(G) = \prod_{e=uv\in E(G)}(d(u)d(v))$

$= \prod_{e=uv\in E(G)}(d(H_i) * d(C_i)) * \prod_{e=uv\in E(G)}(d(C_i) * d(C_j))$

$= \prod_{i=1}^{(2n+2)}(d(H_i) * d(C_i)) * \prod_{i=1}^{(n-1)}(d(c_i) * d(C_i))$

= (1*4)*(1*4)*- - -*(1*4) * ( 4*4)*(4*4)*- - -*(4*4)

$(2n+2)$ times $(n-1)$ times

$= (4)^{(18)} * (16)^{(7)}$

$= (4)^{(18)} * (4)^{(14)} = (4)^{(32)}$

**Theorem XIII**

These new indices are first multiple Zagreb index $PM_1(G)$ and second multiple Zagreb index $PM_2(G)$ and are defined as

**I)** $PM_1(G) = \prod_{e=uv\in E(G)}(d(e)+2)$ and II) $PM_2(G) = \prod_{u\in V(G)}(d(u))^{(d(u))}$

**Proof:** I) $d(u) + d(v) - 2 = d(e)$ where $e = uv \in E(G)$

This implies

$PM_1(G) = \prod_{e=uv\in E(G)}(d(u)+d(v)) = \prod_{e=uv\in E(G)}(d(e)+2)$ (Theorem IV)

II) Let $\{v_1, v_2, v_3, ---, v_{n-1}, v_n\}$ be the set be vertices of a simple graph $G = (V, E)$

With degree sequence

$(d_1, d_2, d_3, ---, d_{n-1}, d_n)$ such that $d(v_i) = d_i$ for $1 \le i \le n$

Consider the pair

$$d(v_i) * d(v_j) = d_i * d_j \quad \text{and}$$

$$\left(d(v_i) * d(v_{j1})\right) * \left(d(v_i) * d(v_{j2})\right) --- * \left(d(v_i) * d(v_{jm})\right) * \text{ --- } * d(v_{n-1}) * \text{---} * d(v_n)$$

This implies for each $1 \le i \le n$, $d(v_i)$ shows exactly $d_i = d(v_i)$ times in the product $PM_2(G) = \prod_{e=uv\in V(G)}(d(u) * d(v))$.

Hence

$\prod_{e=uv\in V(G)}(d(u) * d(v)) = \prod_{u_i\in V(G)}(d(u_i))^{(d(u_i))}$ where $\sum_{i=1}^{n} d(u_i) = 2|E|$ and then $PM_2(G) = \prod_{e=uv\in V(G)}(d(u) * d(v))$ .

**Example VI**

For each edge $e_i = H_iC_i$ , we've $d(e_i) = d(H_iC_i) = 3$ and for each $e_i = C_iC_j$ adjacent carbon atoms $d(e_i) = d(C_iC_j) = 6$ . Combining these,

I) $PM_1(G) = \prod_{e=uv\in E(G)}(d(u)+d(v)) = \prod_{e=uv\in E(G)}(d(e)+2)$

$= \prod_{e=H_iC_i\in E(G)}(d(H_iC_i)+2) * \prod_{e=C_iC_j\in E(G)}(d(C_iC_j)+2)$

$= \prod_{e=H_iC_i\in E(G)}(3+2) * \prod_{e=C_iC_j\in E(G)}(6+2)$

$= \prod_{i=1}^{(2n+2)}(5) * \prod_{i=1}^{(n-1)}(8)$ because #( $H_iC_i$) = ( $2n+2$) and #($C_iC_j$) = $(n-1)$

$= (5)^{(2n+2)} * (8)^{(n-1)}$

$= 625* (200)^{(n-1)}$ (See example VI)

II) $PM_2(G) = \prod_{e=uv\in V(G)}(d(u) * d(v)) = \prod_{u_i\in V(G)}(d(u_i))^{(d(u_i))}$

$= \prod_{H_i\in V(G)}(d(H_i))^{(d(H_i))} * \prod_{C_i\in V(G)}(d(C_i))^{(d(C_i))}$ because $d(H_i) = 1$

$= \prod_{C_i\in V(G)}(d(C_i))^{(d(C_i))} = \prod_{C_i\in V(G)}(4)^{(4)} = \prod_{i=1}^{n} 4^4$

$= (4^4)^n = (4^4)^{(8)} = (4)^{(32)}$ . (See example VI)

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