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# The Zagreb group indices and polynomials

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***ABSTRACT:-*** Several topological indices are studied for molecular graphs. Topological indices are numerical parameters of a graph which are invariant under graph isomorphisms. The indices of Zagreb group and their polynomials are investigated in this paper.

***Keywords:-*** Molecular graph, degree, eccentricity, topological indices, Zagreb indices, Zagreb polynomials.

## I. INTRODUCTION

Graph theory is one of the hot areas of modern mathematics which has witnessed a magnificent growth due to a number of applications in computer and communication, molecular physics and chemistry, social networks, biological sciences, computational linguistics and in other numerous areas [1].Let G be a simple molecular graph without directed, multiple edges and without loops, the vertex and edge sets of which are represented by V(G) and E(G) respectively. Topological indices are the numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity [2].Topological indices are designed basically by transforming a molecular graph into a number [3]. The distance is an important tool in studying the structure of a graph and plays also dominant role in applications of graph theory [4].

The Zagreb indices belong among the old and most studied molecular structure descriptors and found noteworthy applications in chemistry. "By recent literature search we found 90 papers whose title contain Zagreb index or Zagreb indices, in which count are included papers labeling with augmented, general, modified, reformulated, multiplicative, variable Zagreb indices ,Zagreb co-indices and Zagreb eccentricity index''[5].When a new topological index is introduced in mathematical chemistry ,one of the important questions that need to be answered is for which members of a certain class of n-vertex (chemical or molecular ) graphs this index assumes minimal and maximal values [6].A polynomial of graph is related with construction of graph, which is invariant under graph automorphism. It is easy to see that every polynomial defines a topological index [7]. Hosaya polynomial, Schultz polynomial and modified Schultz polynomial, first and second Zagreb polynomials are studied in many papers.

The Zagreb indices are found to have applications in QSPR and QSAR studies. We define Augmented-Zagreb polynomial and Hyper-Zagreb polynomial and compute the corresponding Zagreb indices for 2-methylbutane.

The aim of this paper is to compute the Zagreb group indices and Zagreb polynomials for a molecular graph of 2-methyl butane.

## II. EXPERIMENTAL PROCEDURE

Any connected graph with maximum degree not extending 4 is called molecular graph. Let G be a simple graph without directed, multiple edges and without loops, the vertex and edge sets of which are represented by V(G) and E(G) respectively. A molecular graph is constructed by representing each atom of a molecule by a vertex and bond between atoms by edges. The distance between the vertices u and v of V(G) is denoted by d(u,v) and it is defined as the number of edges in a minimal path connecting the vertices u and v. The degree of a vertex v of graph is the number of vertices of G adjacent to it and denoted by dG(v) or simply as dv .The vertex degree in any molecular graph has 1, 2, 3 or 4 values. For a given vertex u of V(G), its eccentricity ec(u), is the largest distance u and any other vertex v of G [8]. The molecular graph of 2-methylbutane is shown in figure (1). The distance matrix D(G) for
2-merthylbutane is represented in figure (2).

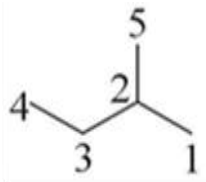


**Fig.1.** Hydrogen suppressed molecular graph of 2-methylbutane.

| | **1** | **2** | **3** | **4** | **5** |
|---|---|---|---|---|---|
| **1** | 0 | 1 | 2 | 3 | 2 |
| **2** | 1 | 0 | 1 | 2 | 1 |
| **3** | 2 | 1 | 0 | 1 | 2 |
| **4** | 3 | 2 | 1 | 0 | 3 |
| **5** | 2 | 1 | 2 | 3 | 0 |

**Fig.2.**Distance matrix D(G) for 2-methylbutane.

## III. RESULTS AND DISCUSSION

The Zagreb group of indices and Zagreb polynomials are discussed in this section. Our notations are standard and mainly taken from [9-12].

### 3.1 Zagreb polynomials and their corresponding indices:

The Zagreb first, second, third and modified second polynomials their corresponding Zagreb indices are degree-based and are defined as:

$M_1(G, x) = \sum_{uv \in E(G)} x^{du+dv}$, $M_2(G, x) = \sum_{uv \in E(G)} x^{du*dv}$,

$M_3(G, x) = \sum_{uv \in (E)} x^{|du - dv|}$ and $M_2*(G, x) = \sum_{uv \in (E)} x^{(1/du*dv)}$,

And the corresponding Zagreb indices are:

$M_1(G) = \frac{\partial M1(G,x)}{\partial x}\big|_{x=1}$, $M_2(G) = \frac{\partial M2(G,x)}{\partial x}\big|_{x=1}$, $M_3(G) = \frac{\partial M3(G,x)}{\partial x}\big|_{x=1}$ and

$M_2^*(G) = \frac{\partial M^*2(G,x)}{\partial x}\big|_{x=1}$.

Where $d_u$, $d_v$ are the vertex degree for any two adjacent vertices and x is dummy variable. The degree for vertices 1, 2, 3, 4 and 5 in 2-methylbutane are 1,3,2,1 and 1 respectively. The first Zagreb index is computed from fig. (1) by considering degrees and edges of graph (G) 2-methylbutane through both approaches.

$M_1(G, x) = x^5 + 2x^4 + x^3$, $M_1(G) = \frac{\partial M1(G,x)}{\partial x}\big|_{x=1}$ = 5+8+3 = 16, and $M_1(G)$ = 5+2*4+3 = 16.

### 3.2 Hyper-Zagreb polynomial and Augmented-Zagreb polynomial

We define Hyper-Zagreb polynomial and Augmented-Zagreb polynomial [7] and their corresponding indices and we compute them for 2-methylbutane. The values of these polynomials and indices are reported in table no. (1).

$HM(G, x) = \sum_{uv \in E(G)} x^{(du+dv)^2} = x^{25} + 2x^{16} + + x^9$

$AZ(G, x) = \sum_{uv \in E(G)} x^{[(du*dv)/(du+dv-2)]^3} = 2x^2 + 2x^{3/2}$

And the corresponding indices as

$HM(G) = \frac{\partial HM(G,x)}{\partial x}\big|_{x=1}$ = 25+32+9 = 66 and $AZI(G) = \frac{\partial AZ(G,x)}{\partial x}\big|_{x=1}$ = 27+16+5 = 07.

### 3.3 Multiplicative and eccentricity version of Zagreb indices

The multiplicative and eccentricity version of Zagreb indices are defined as follows. The multiplicative version of Zagreb indices and eccentricity versions are computed for

2-methyl butane and given in table no. (2).The maximum distance, max $d(v,v_i)$ from a given vertex v to any other vertex $v_i$ occurs only when $v_i$ is a pendant vertex. With this observation the eccentricities of the five vertices (fig.1) are ec(1) = 3,ec (2) = 2,ec(3) = 2,ec(4) = 3 and ec(5) = 3 [9,10].

First multiplicative Zagreb index: $\Pi_1(G) = \prod_v dv(G)^2$

Second multiplicative Zagreb index: $\Pi_2(G) = \prod_{uv \in (G)} (du\ dv)$

Second multiplicative eccentricity Zagreb index: $\Pi_2^*(G) = \prod_{uv \in E(G)} (ec(u)ec(v))$

Third multiplicative eccentricity Zagreb index: $\Pi_3^*(G) = \prod_{uv \in E(G)} (ec(u) + ec(v))$

Multiplicative sum Zagreb index: $\Pi_1^*(G) = \prod_{uv \in E(G)} [d(u) + d(v)]$.

**3.4 Fourth and sixth Zagreb polynomials and corresponding indices**

The fourth and sixth polynomials and their corresponding indices are eccentricity based which are defined as:

Fourth Zagreb polynomial: $Z_{g\,4}(G, x) = \sum_{u\,v \in E(G)} x^{[ec(u)+ec(v)]}$

Sixth Zagreb polynomial: $Z_{g\,6}(G, x) = \sum_{u\,v \in E(G)} x^{[ec(u)\ ec(V)]}$

Fourth Zagreb index: $Z_{g\,4}(G) = \sum_{u\,v \in E(G)} (ec(u) + ec(v))$

Sixth Zagreb index: $Z_{g\,6}(G) = \sum_{u\,v \in E(G)} (ec(u)ec(v))$

**3.5 Inequality in Zagreb indices**

For all simple graphs G with n vertices and m edges the Zagreb indices inequalities are

[13]: (1) $\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m}$ and (2) $M_1 + 2\,M_2 \leq 4\,m^2$, n = 5, m = 4, both these inequalities are observed for molecular graph of 2-methylbutane as $3.2 \leq 3.5$ and $44 \leq 64$.

The Zagreb group of indices are computed from first derivative of the corresponding Zagreb polynomial at x = 1 and from the respective formulas of Zagreb indices [14].The Zagreb group indices computed from formula and first derivative of polynomial at x = 1 yield the same value. These values are reported in the table no. (1). For this molecular graph $\Pi_2^*(G)$ has highest value and $M_2^*(G)$ has least value among the Zagreb indices studied. The order followed among Zagreb group indices is $\Pi_2^*(G) > \Pi_3^*(G) > \Pi_1(G) \geq \Pi_1^*(G) > \Pi_2(G) >$ HMI (G)$> Z_{g\,6}(G) > Z_{g\,4}(G) > M_1(G) > M_2(G) >$ AZI(G) $> M_3(G) > M_2^*(G)$.

**Table no. (1):** The values of Zagreb group of indices and polynomials for 2-methyl butane.

| Zagreb indices | Values of indices | Polynomials |
|---|---|---|
| $M_1(G)$ | 16 | $X^5+ 2x^4+ x^3$ |
| $M_2(G)$ | 14 | $X^6+ 2x^3+ x^2$ |
| $M_3(G)$ | 06 | $2\,x^2+ 2x^1$ |
| $M_2^*(G)$ | 1.333 | $2\,x^{1/3}+ x^{1/2}+ x^{1/6}$ |
| HMI(G) | 66 | $x^{25}+2x^{16}+ x^9$ |
| AZI(G) | 07 | $2x^2+2x^{3/2}$ |
| $Z_{g4}(G)$ | 19 | $3X^5+ x^4$ |
| $Z_{g6}(G)$ | 22 | $3X^6+ x^4$ |

**Table no. (2):** Multiplicative versions of Zagreb indices for 2-methyl butane.

| Zagreb indices | Values of indices |
|---|---|
| $\Pi_1(G)$ | 240 |
| $\Pi_2(G)$ | 108 |
| $\Pi_2^*(G)$ | 864 |
| $\Pi_3^*(G)$ | 500 |
| $\Pi_1^*(G)$sum-modified | 240 |

## IV. CONCLUSIONS

The matrix representation of molecular graph is used to study topological indices. The vertex-degree and eccentricity-based Zagreb group indices and polynomials are studied for molecular graph. The values for first and second Zagreb indices computed from formula and polynomial are the same. Hyper-Zagreb index and Augmented-Zagreb index are computed from Hyper-Zagreb Polynomial and Augmented-Zagreb polynomial respectively.

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