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Note on multiple Zagreb indices

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ABSTRACT

The Zagreb indices are the oldest graph invariants used in mathematical chemistry to predict the chemical phenomena. In this paper we define the multiple versions of Zagreb indices based on degrees of vertices in a given graph and then we compute the first and second extremal graphs for them.

Keywords: Zagreb indices, vertex degree, multiple Zagreb indices.

1. INTRODUCTION

All graphs considered in this paper are simple and connected. Our notation is standard and mainly taken from standard books of graph theory such as, e. g., [1]. A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. If e is an edge of G, connecting the vertices u and v, then we write $e = uv$ and say "u and v are adjacent". The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively.

A ***connected graph*** is a graph such that there is a path between all pairs of vertices. The degree dv of a vertex $v \in (G)$ is the number of vertices of G adjacent to v. A vertex $v \in (G)$ is said to be isolated, pendent, or fully connected if $dv = 0$; $dv = 1$, or $dv = n$-1, respectively. The n-vertex graph in which all vertices are fully connected is the complete graph K_n. The n-vertex graph with a single fully connected vertex and n - 1 pendent vertices is the star S_n. The connected n-vertex graph with two pendent vertices and n-2 vertices of degree 2 is the path P_n. The connected n-vertex graph whose all vertices are of degree 2 is the cycle C_n.

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Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular graph using mathematical ways without referring to quantum mechanics [2-4]. ***Chemical graph theory*** is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena. This theory plays a significant influence on the enlargement of the chemical sciences [5, 6].

A ***molecular graph*** is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. By IUPAC terminology, a ***topological index*** is a numerical value for correlation of chemical structure with various physical properties, chemical reactivity or biological activity.

The aim of this paper is to put forward a new variant of the **Zagreb indices**. We determined their basic properties and characterize graphs extremal with respect to them.

2. RESULTS AND DISCUSSION

The first and second Zagreb descriptors are among the oldest graph invariants, defined in 1972 by Gutman and his co-authors [7], and are given different names such as the Zagreb group indices, the Zagreb group parameters and most often, the Zagreb indices. They are defined as:

$$M_1(G) = \sum_{uv\in E(G)}(du + dv) \text{ and } M_2(G) = \sum_{uv\in E(G)}(du \times dv).$$

Here by using definition of Zagreb indices we define two new topological indices based on degree of vertices and we name it ***multiple Zagreb*** indices. These topological indices are defined as [8-11]:

$$PM_1(G) = \prod_{uv\in E(G)}(du + dv) \text{ and } PM_2(G) = \prod_{uv\in E(G)}(du \times dv).$$

Example 1. Suppose S_n be the star graph on n vertices. The degree of the central vertex is $n - 1$ and other vertices have degree one. This implies

$$PM_1(S_n) = n^{n-1}.$$

Example 2. Let K_n be a complete graph on n vertices. The degree of any vertex is n - 1 and so

$$PM_1(K_n) = (2n-2)^n \frac{(n-1)}{2}.$$

Example 3. Consider the path P_n with n vertices. The degree of end vertices is 1 and other vertices have degree two. Hence,

$$PM_1(P_n) = 9.4^{n-3}.$$

Example 4. Consider the cycle C_n with n vertices. Since every vertex is of degree 2, then

$$\mathrm{PM}_1(\mathrm{C}_n) = 4^n.$$

Theorem 5. Let G be an arbitrary n vertices graph. Then

$$PM_1(G) \leq PM_1(K_n).$$

Theorem 6.

(a) The n-vertex tree with maximal first multiple Zagreb index is the star S_n. The value of first multiple Zagreb index for this graph is $PM_1(S_n) = n^{n-1}$.
(b) The n-vertex connected unicyclic graph with maximal first multiple Zagreb index is $S_n + e$, with $PM_1(S_n + e) = 4\,(n+1)^2 n^{n-3}$, see Figure 1.
(c) Among all bicyclic graphs on n vertices, graph G, depicted in Figure 2, has the maximal first multiple Zagreb index. The value of first multiple Zagreb index for this graph is

$$5^2 \times (n+1)^2 \times (n+2) \times n^{n-4}.$$

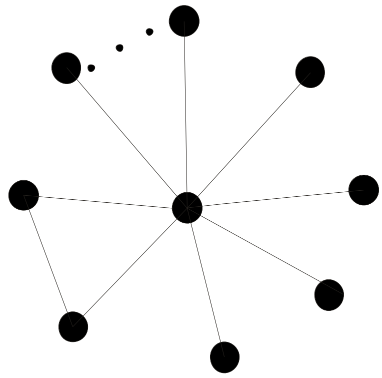

Figure 1. The Graph $S_n + e$.

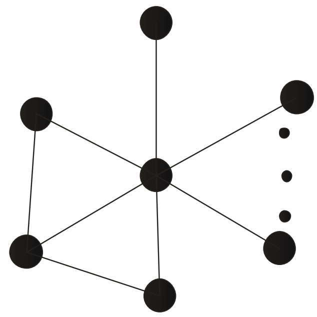

Figure 2. The Graph G.

Theorem 7.

(a) The n-vertex tree with minimal first multiple Zagreb index is the path P_n in which $PM_1(P_n) < PM_1(T)$.
(b) The n-vertex connected unicyclic graph with minimal first multiple Zagreb index is C_n.
(c) Among all bicyclic graphs on n vertices, graph H, depicted in Figure 3, has the minimal first multiple Zagreb index. The value of first multiple Zagreb index for this graph is $PM_1(H_n) = 5^4.6.4^{n-4}$.

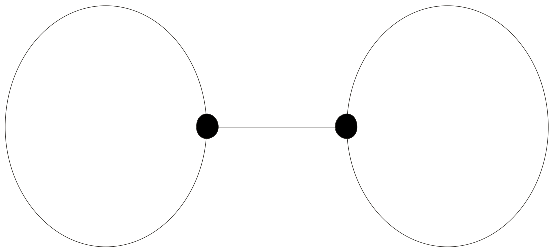

Figure 3. The Graph H.

Theorem 8.

(a) The n-vertex tree with second maximal first multiple Zagreb index is the graph S'_n depicted in Figure 4. The value of first multiple Zagreb index for this graph is $3n(n-1)^{n-3}$.

(b) The n-vertex connected unicyclic graph with second maximal first multiple Zagreb index is graph $K = S_n + e + \acute{e}$, depicted in Figure 5. The value of first multiple Zagreb index for this graph is

$$PM_1(S_n + e + \acute{e}) = 4^2n^2(n-1)^{n-4}.$$

(c) Among all bicyclic graphs on n vertices, the graph F, depicted in Figure 6 has the second maximal first multiple Zagreb index. The value of first multiple Zagreb index for this graph is $100 \times (n + 1) \times n^2 \times (n - 1)^{n-5}$.

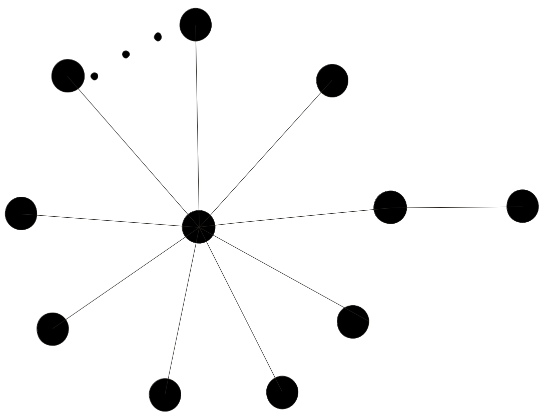

Figure 4. The Graph S'_n.

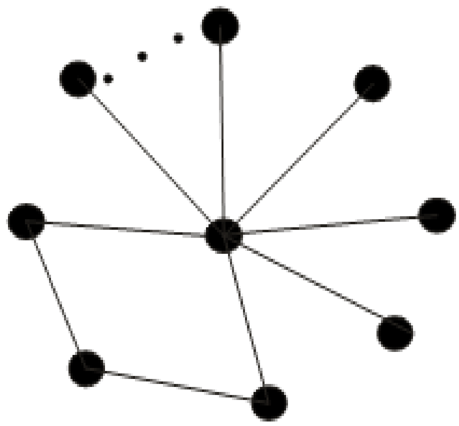

Figure 5. The Graph $S_n + e + e'$.

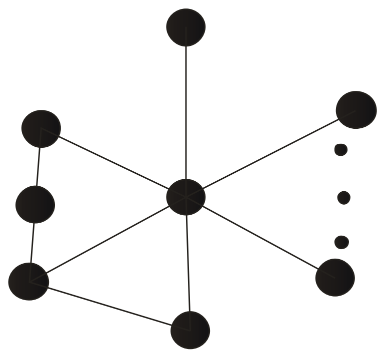

Figure 6. The Graph F.

Theorem 9.

(*a*) The n-vertex tree with second minimal first multiple Zagreb index is the graph Q, depicted in Figure 7. The value of the first multiple Zagreb index for this graph is $3^2 \times 5^2 \times 4^{n-5}$

(*b*) The n-vertex connected unicyclic graph with second minimal first multiple Zagreb index is graph R, depicted in Figure 8. The value of first multiple Zagreb index for this graph is $5^3 \times 3 \times 4^{n-4}$.

(*c*) Among all bicyclic graphs on n vertices, the graph S, depicted in Figure 9 has the second minimal first multiple Zagreb index. The value of first multiple Zagreb index for this graph is $5^6.4^{n-5}$.

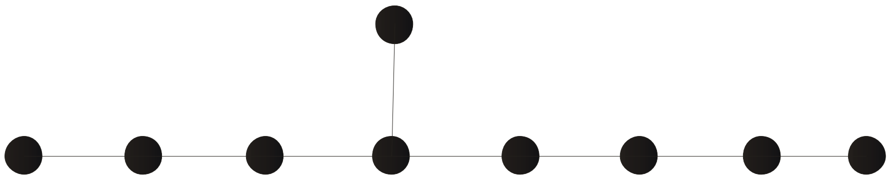

Figure 7. The Graph *Q*.

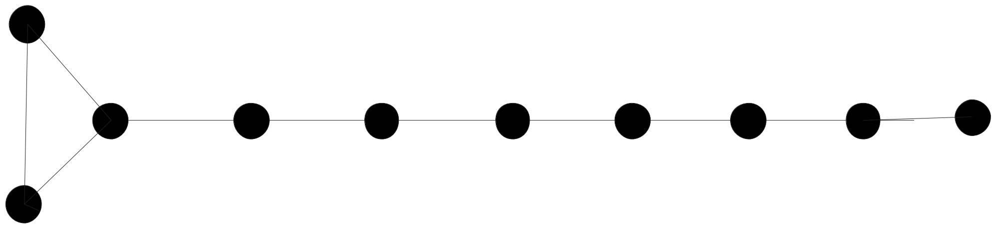

Figure 8. The Graph *R*.

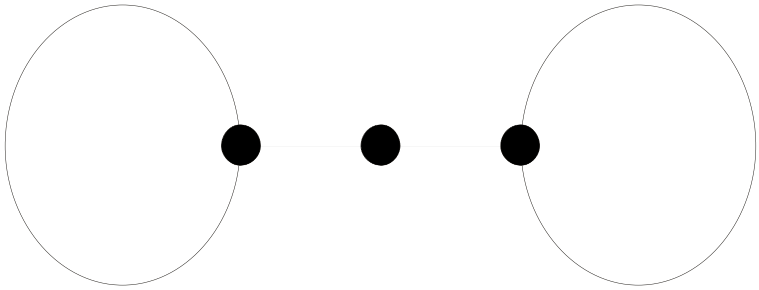

Figure 9. The Graph *S*.

3. CONCLUSIONS

By using the definition of the multiple Zagreb indices, we computed the extremal graphs respect to these new topological indices.

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