MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **65** (2011) 85-92

ISSN 0340 - 6253

Extremal Graphs with Respect to the Zagreb Coindices

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(Received July 11 , 2009)

Abstract

Recently introduced Zagreb coindices are a generalization of classical Zagreb indices of graphs. In this paper we determine the extremal values of these new topological invariants over some special classes of graphs. The extremal graphs are also presented.

1 Introduction

A **graph invariant** is any function on a graph that does not depend on a labeling of its vertices. Such quantities are also called **topological indices**. Hundreds of different invariants have been employed to date (with unequal success) in QSAR/QSPR studies. Among more useful of them appear two that are known under various names, but mostly as Zagreb indices. Due to their chemical relevance they have been subject of numerous papers in chemical literature [2, 9, 10, 11, 15, 19], while the first Zagreb index, also attracted a significant attention of mathematicians. One of the focal points of their research has been the problem of determining their extremal values and the corresponding extremal graphs [3, 4, 5, 14]. The aim of this paper is to investigate similar problems for a recently introduced generalization of Zagreb indices.

2 Definitions and preliminaries

All graphs in this paper are finite and simple. For terms and concepts not defined here we refer the reader to any of several standard monographs such as, e.g., [6] or [17].

Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. For every vertex $u \in V(G)$, the edge connecting u and v is denoted by uv and $\delta_G(u)$ denotes the degree of u in G. We will omit the subscript G when the graph is clear from the context.

The Zagreb indices were originally defined as follows:

$$M_1(G) = \sum_{u \in V(G)} \delta(u)^2$$

$$M_2(G) = \sum_{uv \in E(G)} \delta(u)\delta(v) \ .$$

Here $M_1(G)$ and $M_2(G)$ denote the first and the second Zagreb index, respectively. The first Zagreb index can be also expressed as a sum over edges of G,

$$M_1(G) = \sum_{uv \in E(G)} [\delta(u) + \delta(v)] \ .$$

We refer the reader to [15] for the proof of this fact. The readers interested in more information on Zagreb indices can be referred to [2, 9, 10, 11, 12, 19].

The Zagreb indices can be viewed as the contributions of pairs of adjacent vertices to certain degree-weighted generalizations of Wiener polynomials [12]. It turned out that computing such polynomials for certain composite graphs depends on such contributions from pairs of non-adjacent vertices. That prompted introduction of Zagreb coindices in reference [7].

The **first Zagreb coindex** of G is defined by

$$\overline{M}_1(G) = \sum_{uv \notin E(G)} [\delta(u) + \delta(v)]$$

and the **second Zagreb coindex** is given by

$$\overline{M}_2(G) = \sum_{uv \notin E(G)} [\delta(u)\delta(v)] \ .$$

For the sake of completeness we state here some results of references [1, 16, 18] and [20] which will be useful throughout the paper.

A sequence $\delta_1 \geq \delta_2 \geq \cdots \geq \delta_n$is called the **degree sequence** of a graph G if there exists a labeling $\{v_1, \ldots, v_n\}$ of vertices of G such that $\delta_1 = \delta(v_1)$, $\ldots$, $\delta_n = \delta(v_n)$.

The girth of G is the length of a shortest cycle contained in G. We assume that $N_i(v) = \{w \in V(G) \mid d(v,w) = i\}$, where $d(v,w)$ is the length of a shortest path connecting v and w. Define $n_i(v) = |N_i(v)|$. The **eccentricity** $\varepsilon(v)$ of v is defined as $\varepsilon(v) = \max_{w \in V(G)}\{d(v,w)\}$. The **radius** $r = r(G)$ and the **diameter** $D = D(G)$ are defined as the minimum and maximum of $\varepsilon(v)$ over all vertices $v \in V(G)$. A **Moore graph** is a graph of diameter k with girth $2k+1$. Those graphs have the minimum number of vertices possible for a regular graph with given diameter and maximum degree.

Lemma A. [1]
Suppose G is a connected graph. Then we have:

(a) $\overline{M}_1(G) = 2m(n-1) - M_1(G)$

(b) $\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G)$. ■

Reference [16] is concerned with degree-distances in unicyclic and bicyclic graphs. The following result will be useful in establishing bounds and extremal graphs for Zagreb coindices over such graphs.

Lemma B. [16]
(a) Let $n \geq 3$. The integers $\delta_1 \geq \cdots \geq \delta_n \geq 1$ are degrees of the vertices of a unicyclic graph if and only if their sum is equal to $2n$ and at least three of them are greater or equal to 2.
(b) Let $n \geq 4$. The integers $\delta_1 \geq \cdots \geq \delta_n \geq 1$ are degrees of the vertices of a bicyclic graph G if and only if their sum is equal to $2n+2$, at least four of them are greater than two, and $\delta_1 \leq n-1$. ■

Reference [18] gives upper and lower bounds on the Zagreb indices over triangle- and quadrangle-free graphs. Our results on extremal values and graphs for Zagreb coindices of such graphs will depend on the following results.

Lemma C. [18]
(a) Let G be a connected graph. Then

$$M_1(G) \geq 2m + \sum_{v \in V(G)} n_2(v)$$

$$M_2(G) \geq \frac{1}{2} M_1(G) + \frac{1}{2} \sum_{v \in V(G)} \delta(v) n_2(v) \ .$$

The equalities hold if and only if G is a triangle- and quadrangle-free graph.

(b) Let G be a triangle- and quadrangle-free graph on n vertices and m edges with radius r. Then $M_1(G) \leq n(n+1-r)$ and $M_2(G) \leq m(n+1-r)$. The equality is valid if and only if G is a Moore graph of diameter 2 or $G = C_6$. ■

We conclude this section by quoting relevant results from reference [21] concerned with bounds on the Zagreb indices of series-parallel graphs. A graph is called **series-parallel** if it does not contain K_4 as a minor; equivalently, it does not contain a subdivision of K_4 [8].

Lemma D (Theorems 1 and 3 of [20])

Let G be a series-parallel graph with n vertices and m edges without isolated vertices. Then

$$\begin{aligned} M_1(G) &\leq n(m-1) + 2m \\ M_2(G) &\leq m^2 + \frac{1}{2} n(m-1) \end{aligned}$$

with equality for $n \geq 3$ if and only if G is isomorphic to $K_{1,1,n-2}$. ■

In the above Lemma $K_{1,1,n-2}$ denotes the complete tripartite graph on n vertices with partition classes of sizes 1, 1, and $n-2$.

3 Main Results

It is easy to see that $M_1(C_n) = 4n$ for $n \geq 3$. Also, $M_1(P_1) = 0$ and $M_1(P_n) = 4n - 6$ for $n > 1$. Let $\mathcal{T}_n$ and $\mathcal{G}_n$ denote the set of all $n-$vertex trees and $n-$vertex connected graphs, respectively. If $G \in \mathcal{G}_n$ then $M_1(G) \leq n(n-1)^2$, with equality if and only if G is isomorphic to a complete graph K_n. Obviously, the path P_n and the star S_n have the minimum and maximum M_1 in $\mathcal{T}_n$, respectively. On the other hand, if H is a subgraph of G then $M_1(H) \leq M_1(G)$. Therefore, the minimum of M_1 on the set of all connected graphs with n vertices is the same as the minimum of M_1 on $\mathcal{T}_n$. This implies that P_n and K_n have the minimum and maximum Zagreb index M_1 on $\mathcal{G}_n$.

The aim of this section is to obtain the extremal graphs with respect to the Zagreb coindices. We first consider $M_1(G)$. In particular, we will prove that for all $T \in \mathcal{T}_n$, $\overline{M}_1(S_n) \leq \overline{M}_1(T) \leq \overline{M}_1(P_n)$. The results of the same type will be also established for the classes of unicyclic and bicyclic graphs.

Lemma 1. If $T \in \mathcal{T}_n$ then $\overline{M}_1(S_n) \leq \overline{M}_1(T) \leq \overline{M}_1(P_n)$.

Proof. This is an immediate consequence of Lemma A (a) and the first paragraph of this section. ■

Suppose $\mathcal{G}_n^1$ denotes the set of all $n-$vertex unicyclic graphs.

Lemma 2. If $G \in \mathcal{G}_n^1$ then $(n+2)(n-3) \leq \overline{M_1}(G) \leq 2n(n-3)$. Moreover, the left and right equalities hold if and only if G is isomorphic to $K_{1,n-1}+e$ and C_n, respectively.

Proof. Since the sum of degrees in G is equal to $2n$, by Lemma B (a) $M_1(G)$ attains its maximum on $\mathcal{G}_n^1$ if and only if $\delta_1 = n-1$, $\delta_2 = \delta_3 = 2$ and $\delta_4 = \cdots = \delta_n = 1$, i. e., $G \cong K_{1,n-1}+e$. Therefore, $M_1(G) \leq n^2-n+6$. By Lemma A (a), $n^2-n-6 \leq \overline{M_1}(G)$. On the other hand, $M_1(G)$ attains its minimum on $\mathcal{G}_n^1$ if and only if every vertex of G has degree 2. Therefore, $M_1(G) \geq 4n$ and by Lemma A (a), $\overline{M_1}(G) \leq 2n^2-6n$. ■

Let $\mathcal{G}_n^2$ denote the set of all $n-$vertex bicyclic graphs. Such graphs have obviously $n+1$ edges.

Lemma 3. If $G \in \mathcal{G}_n^2$ then $n^2+n-16 \leq \overline{M_1}(G) \leq 2n^2-4n-12$. The left equality is satisfied if and only if G is isomorphic to $K_{1,n-1}+e+f$, where e and f are two edges with a common vertex forming two adjacent triangles in $K_{1,n-1}$. The right equality is satisfied if and only if G is isomorphic to a graph constructed from C_p and C_q joined by a path P_{n-p-q}, $3 \leq p, q \leq n-3$.

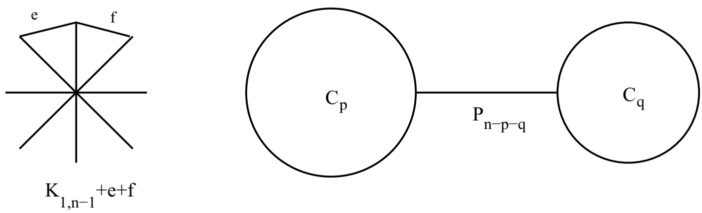

Figure 1: Extremal graphs for Lemma 3.

Proof. Since the sum of degrees is $2n+2$, by Lemma B (b) the maximum is attained if and only if $\delta_1 = n-1$, $\delta_2 = \delta_3 = 2$, $\delta_4 = 3$ and $\delta_5 = \cdots = \delta_n = 1$. Therefore, $M_1(G) \leq n^2-n+14$ and so $n^2+n-16 \leq \overline{M_1}(G)$. On the other hand, the minimum of $M_1(G)$ on $\mathcal{G}_n^2$ is attained on a graph with the degree sequence $\delta_1 = \delta_2 = 3$ and $\delta_3 = \cdots = \delta_n = 2$. Such graphs are constructed from two cycles C_p and C_q by connecting them by a path of length $n-1-p-q$. This implies that $M_1(G) \geq 4n+10$ and so $\overline{M_1}(G) \leq 2n^2-4n-12$, proving the lemma. ■

The extremality results for $M_1(G)$ for unicyclic and bicyclic graphs can be also derived from results of [13] as reported in [21].

Let us now turn our attention to $\overline{M}_2(G)$. Starting from the extremal trees for $M_2(T)$ as reported in [5] and formula

$$\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G)$$

from Lemma A (b) it is easy to see that for an $n-$vertex tree T, $\overline{M_2}(S_n) \leq \overline{M_2}(T) \leq \overline{M_2}(P_n)$.

Let us now look at more general graphs. If a connected graph G is triangle- and quadrangle-free, we can use the results of reference [18] summarized in Lemma C to obtain both upper and lower bounds on $\overline{M}_2(G)$.

Lemma 4. Suppose G is a triangle- and quadrangle-free connected graph with n vertices, m edges and radius r. Then $\overline{M_2}(G) \geq 2m^2-(n+1-r)(m+\frac{1}{2}n)$ with equality if and only if G is a Moore graph of diameter 2 or $G \cong C_6$.

Proof. The proof is straightforward and follows from Lemma C (b) and Lemma A (b). ■

The upper bound follows by the same reasoning from Lemma A (b) and Lemma C (a).

Lemma 5. Suppose G is a connected graph. Then

$$\overline{M_2}(G) \leq 2m^2 - \frac{1}{2}\sum_{v\in V}\delta(v)(\delta(v)+n_2(v)) - \frac{1}{2}\sum_{v\in V}(\delta(v)+n_2(v)).$$

The equality holds if and only if G is a triangle- and quadrangle-free connected graph. ■

For a triangle- and quadrangle-free connected graph, we have the following identity between $\overline{M}_1(G)$ and $\overline{M_2}(G)$.

$$\overline{M_2}(G) = \overline{M}_1(G) + 2m(m-n+1) - \frac{1}{2}\sum_{v\in V(G)}\delta(v)n_2(v).$$

This identity is analogous to the identity

$$M_2(G) = \frac{1}{2}\left[M_1(G) + \sum_{v\in V(G)}\delta(v)n_2(v)\right]$$

of reference [18]. For trees this further reduces to

$$\overline{M}_2(G) = \overline{M}_1(G) - \frac{1}{2} \sum_{v \in V(G)} \delta(v) n_2(v) \ .$$

We conclude the section with a result concerned with series–parallel graphs.

Lemma 6. Suppose G is a series-parallel graph without isolated vertices. Then $\overline{M_1}(G) \geq m(n-4)+n$ and $\overline{M_2}(G) \geq (m-n)(m-1)$. The equality holds if and only if $G \cong K_2, K_{1,1,n-2}$. ■

The proof follows from Lemma A and Lemma D, and we omit it.

4 Concluding remarks

It would be interesting to extend the presented results also to some other classes of graphs of chemical interest. Our results leave open the question of the minimum values of Zagreb coindices over chemical trees. Another interesting class is formed by unbranched polymers such as, e.g., benzenoid chains. At the present we are not aware of any results of this type.

Acknowledgment. Partial support of the Ministry of Science, Education and Sport of the Republic of Croatia (Grants No. 037-0000000-2779 and 177-0000000-0884) is gratefully acknowledged. The first author was supported in part by a grant from IPM (No. 88200124).

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