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On Discriminativity of Zagreb Indices

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ABSTRACT

Zagreb indices belong to better known and better researched topological indices. We investigate here their ability to discriminate among benzenoid graphs and arrive at some quite unexpected conclusions. Along the way we establish tight (and sometimes sharp) lower and upper bounds on various classes of benzenoids.

Keywords: Zagreb index, benzenoid graph, catacondensed benzenoid.

1. INTRODUCTION

Central paradigm of chemical graph theory is the belief that valuable information about physico-chemical properties of various organic molecules can be obtained from topological aspects of their structure. The molecules are represented by suitably defined graphs, and various graph-theoretic invariants of those graphs are then defined and studied. Those that exhibit a significant correlation with some property are then elevated to the status of topological indices and (usually) attract a lot of attention in both mathematical and chemical community. Among the better known examples are the Wiener index, the Szeged index, and also two invariants introduced some forty years ago known as the Zagreb indices.

One of the most valuable and sought after qualities of topological indices is their discriminativity, i.e., the ability to assign distinct values to non-isomorphic graphs. It is well known that no invariant can achieve the perfect discriminativity; for large enough graphs it inevitably happens that two non-isomorphic graphs have the same value of the topological index. It might happen that for some classes of graphs the discriminativity is preserved longer than for some other classes; if that happens for a chemically interesting class, the topological index receives an additional boost in popularity.

The Zagreb indices, mentioned above, doubtless belong to more popular invariants. Due to their chemical relevance they have been studied in numerous papers in chemical literature [2, 8, 9, 10, 13, 17]. They have also attracted significant attention from the mathematicians [3, 5, 6, 12, 15, 16]. Another topic that frequently appears in papers by both

mathematicians and chemists are the so called benzenoid graphs. The chemists study them as the models for benzenoid hydrocarbons, while the mathematicians see them as the finite pieces of hexagonal tilings. The literature on benzenoid graphs is vast; the results have been accumulating since the middle of the past century. An interested reader can find a good starting point in a monograph concerned mostly with the enumeration of matchings in such graphs [4].

Given the popularity of both subjects, one could expect that there are plenty of papers dealing with Zagreb indices of benzenoid graphs. That does not seem to be true. One of the reasons might be that, surprisingly, Zagreb indices do not discriminate well among benzenoid graphs. The goal of this paper is to provide a proof of the above claim and to investigate some consequences.

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., [14].

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 $\delta(u)$ denotes the degree of u in G. The *Zagreb indices are 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 [13] for the proof of this fact. We find this definition more useful than the original one. The readers interested in more information on Zagreb indices can also wish to consult [2, 8, 9, 10, 11, 17].

A **hexagonal system** is a collection of congruent regular hexagons arranged in a plane in such a way that two hexagons are either completely disjoint or have a common edge. Such objects appear in mathematical and chemical literature also under many other names, such as hexagonal systems, polyhexes, honeycomb systems, hexagonal animals and hexagonal polyominoes. If the interior of a hexagonal system is 1-connected, we call it a **benzenoid system**. The connection between benzenoid hydrocarbons and benzenoid systems is quite straightforward.

To each benzenoid system we assign a **benzenoid graph**, taking the vertices of hexagons as the vertices of the graph, and the sides of hexagons as its edges. The resulting graph is simple, planar, bipartite and all its bounded faces are hexagons. The vertices of a benzenoid graph B lying on the border of the unbounded face are called **external**; other vertices (if any) are **internal**. A benzenoid graph without internal vertices is called **catacondensed**; otherwise it is **pericondensed**. We will denote a benzenoid graph with h hexagons and i internal vertices by $B(h, i)$. It follows by a simple counting argument that $B(h, i)$ has $4h + 2 - i$ vertices and $5h + 1 - i$ edges [4].

3. MAIN RESULTS

3.1. CATACONDENSED BENZENOIDS

We consider first the catacondensed benzenoids. As mentioned above, they do not have internal vertices, $i = 0$. Hence, a catacondensed benzenoid on h hexagons has $4h + 2$ vertices and $5h + 1$ edges. Its h hexagons belong to one of the four possible types, depending on the number and the relative position of the edges they share with other hexagons. If a hexagon shares one edge with another hexagon, it is called **terminal**. If it shares three edges, no two of the shared edges can be incident to the same vertex. Such hexagon is called **branching**. If the two shared edges are parallel, the hexagon is called **straight**, and if they are not parallel, it is called **kinky**. The reasons for such terminology should be clear from the example shown in Fig. 1, where the type of a hexagon is indicated by the capital initial letter. We denote a catacondensed benzenoid on h hexagons by B_h. The number of terminal, branching, straight and kinky hexagons is denoted by T, B, S and K, respectively.

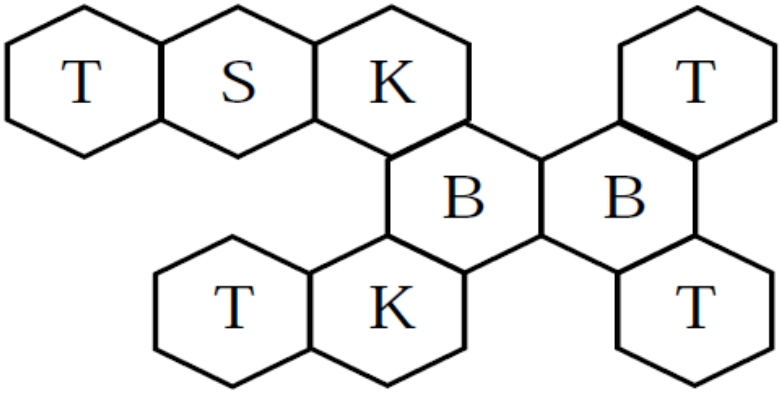

Figure 1: A Catacondensed Benzenoid with Hexagons of Different Types.

Let us call the edges shared by two hexagons internal, and the other edges external. It is clear that each internal edge contributes 6 to $M_1(B_h)$ and 9 to $M_2(B_h)$. Obviously, there are $h-1$ internal edges in B_h, and their collective contribution to $M_1(B_h)$ is given by $6(h-1)$.

Now we proceed to compute the contributions of external edges to $M_1(B_h)$. There are $5h-1-(h-1) = 4h + 2$ external edges in B_h. The terminal hexagons contain $5T$ of them, the branching hexagons contain $3B$, and the remaining hexagons together contain $4(h - T - B)$ external edges. Since the total must sum to $4h+2$, it follows that the number of terminal and the number of branching hexagons are related, $T = B + 2$. The external edges of each terminal hexagon collectively contribute $3\cdot4 + 2\cdot5 = 22$ to $M_1(B_h)$; the three edges of each branching hexagon contribute together $3\cdot6 = 18$. Finally, the contributions of the external edges of both straight and kinky hexagons are both equal to 20 ($4\cdot5$ and $4 + 2\cdot5 + 6$, respectively). Since $S + K = h - T - B = h - 2T - 2$, the total contribution of all external edges to $M_1(B_h)$ is given by

$$22T + 18B + 20(S + K) = 20h + 4.$$

By combining that with the contribution of internal edges we arrive at a surprising conclusion that the first Zagreb index of a catacondensed benzenoid does not depend on the details of its structure; the only thing that matters is the size.

Theorem 1. Let B_h be a catacondensed benzenoid with h hexagons. Then

$$M_1(B_h) = 26h - 2.$$

■

Hence, an index that has been used as a measure of branching for chemical trees cannot distinguish between branched and unbranched benzenoids.

The things are only a bit better for the second Zagreb index. As mentioned, the total contribution of internal edges is given by $9(h - 1)$. For the external edges we readily obtain that the contributions of the hexagons of various types are 24 for T and S, 27 for B and 25 for K. However, the numbers T and S are not related in the way T and B are; hence, we cannot eliminate all structural parameters from the expression for $M_2(B_h)$. We choose to express it in terms of B and S.

Theorem 2. Let B_h be a catacondensed benzenoid with h hexagons. Then

$$M_2(B_h) = 34h - 11 + B - S,$$

where B and S are the number of branching and straight hexagons, respectively.

■

It is immediately clear from the above formula that the second Zagreb index cannot discriminate between the catacondensed benzenoids on h hexagons having the same

number of straight and branching hexagons, such as the pair shown in Fig. 2. Further, it is clear that the minimum value of the second Zagreb index on catacondensed benzenoids is achieved on the benzenoid chain with largest possible number of straight hexagons. Since the largest value of S is $h - 2$, the extremal value is given by $33h - 9$ and the extremal benzenoid is unique, the linear polyacene on h hexagons.

For benzenoid chains, Theorem 2 provides (tight) bounds on the values of second Zagreb index.

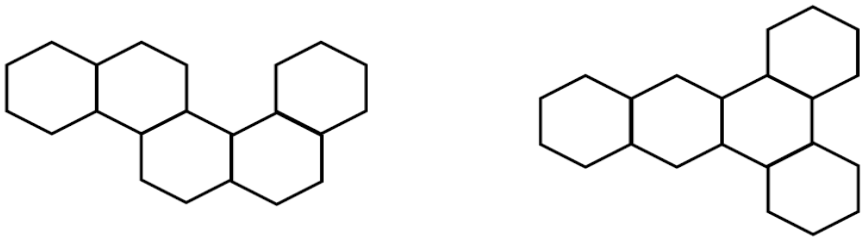

Figure 2: Two Catacondensed Benzenoids with the Same Second Zagreb Index.

Corollary 3. Let B_h be a benzenoid chain on h hexagons. Then

$$33h - 9 \leq M_2(B_h) \leq 34h - 11.$$

■

We see that the second Zagreb index follows a pattern rather common for distance–based invariants, that achieve their extremal values on straight and on nowhere–straight chains.

For branched catacondensed benzenoids, second Zagreb index favors the branching and penalizes the straight hexagons. It follows that the maximum value of $M_2(B_h)$ will be achieved on benzenoids having as many branching hexagons as possible. As the number of branching hexagons cannot exceed $(h - 2)/2$, we obtain the following upper bounds.

Corollary 4. Let B_h be a catacondensed benzenoid on h hexagons. Then

$$33h - 9 \leq M_2(B_h) \leq [69h - 24 - q(h)]/2,$$

where $q(h) = 0$ for an even h and $q(h) = 1$ if h is odd.

■

Since it is always possible to construct a catacondensed benzenoid with $(h-2-q(h))/2$ branching hexagons, the upper bounds are tight. Examples of such benzenoids are shown in Fig. 3.

3.2. PERICONDENSED BENZENOIDS

We have seen that the Zagreb indices, in particular the first one, are poorly suited for discriminating among catacondensed benzenoids. Is the situation any better for the pericondensed case?

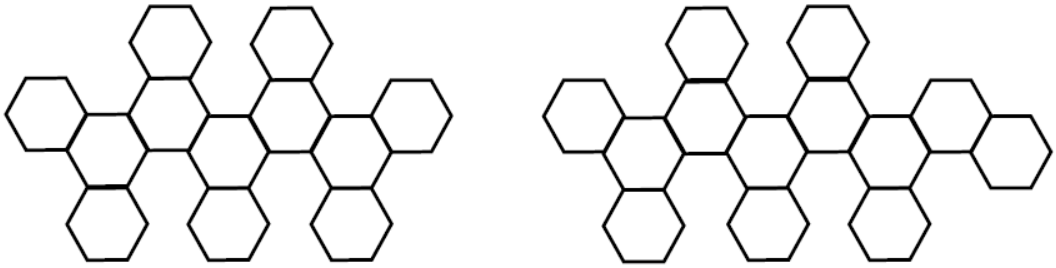

Figure 3: Extremal Catacondensed Benzenoids for the Second Zagreb Index.

Recall that a pericondensed benzenoid on h hexagons with i internal vertices has $4h+2-i$ vertices and $5h + 1 - i$ edges. Since i vertices are internal, that leaves $4h + 2 - 2i$ vertices and the same number of edges on the perimeter of $B(h, i)$. Each of the $h - 1 + i$ internal edges will contribute 6 to $M_1(B(h, i))$ and 9 to $M_2(B(h,i))$. Hence in order to compute the indices, we must determine the contributions of the external edges.

The external edges belong to one of three possible types, depending on the degrees of their end-vertices. We denote the number of external edges with end-vertices of degrees j and k by e_{jk} , for $j, k = 2, 3$.

Lemma 5. $e_{22} = e_{33} + 6$.

Proof. The perimeter of $B(h,i)$ is a simple closed curve in the plane, hence its winding number must be equal to 2π. Start at an external vertex and walk around the perimeter in the counterclockwise direction. Each edge connecting two vertices of degree 3 contributes $-\pi/3$ to the winding number; each edge connecting two vertices of degree 2 contributes $\pi/3$. The remaining edges come in pairs and their contributions cancel, leaving us with

$$2\pi = -\frac{\pi}{3}e_{33} + \frac{\pi}{3}e_{22} ,$$

and the claim follows. ■

Now we can compute $M_1(B(h, i))$. There are $4h + 2 - 2i - 2e_{33} - 6$ external edges connecting vertices of different degrees. Each of them contributes 5 to $M_1(B(h, i))$, and their total contribution to is given by $20h - 10i - 10e_{33} - 20$. By combining this with $6e_{33}$

from the edges with both end-vertices of degree 3 and $4e_{33} + 24$ from the edges connecting two vertices of degree 2, we obtain the total contribution of external edges as $20h-10i+4$. By adding the contribution of internal edges we obtain the following result.

Theorem 6. $M_1(B(h,i)) = 26h - 2 - 4i.$

■

We see that the result does not depend on the number of edges of different types. An immediate consequence is an upper bound on $M_1(B(h, i))$ valid for all benzenoid graphs on a given number of hexagons.

Corollary 7. $M_1(B(h, i)) \leq 26h - 2.$

■

From the subsection on catacondensed benzenoids we know that this bound is tight. To gain some information on the lower bound, we look at benzenoid graphs with many internal vertices. By considering hexagonal benzenoids with p layers of hexagons such as the one shown in Fig. 4, we see that the fraction of internal vertices can be arbitrarily close to one for large enough p. It can be verified by a straightforward computation that H_p has $3p^2 - 3p+1$ hexagons and $6p^2$ vertices, with $6(p - 1)^2$ internal vertices. By plugging those values in the formula of Theorem 6 we obtain $M_1(H_p) = 54p^2-30p$. Now, by dividing this by $3p^2-3p+1$ and expanding the quotient into a power series in $1/p$ at infinity, we obtain

$$\frac{54p^2 - 30p}{3\mathrm{p}^2 - 3\mathrm{p} + 1} = 18 + \frac{8}{p} + \frac{2}{p^2} + \ldots$$

Hence, $M_1(B(h, i)) \geq 18h$, and the lower bound cannot be made any better. The factor 18 does not come as a surprise, reflecting the fact that almost all edges are internal, each of them contributing 3 to both of the hexagons sharing it.

For the second Zagreb index situation is more complicated, due to the fact that the contribution of the external edges with end-vertices of different degrees is not the mean value of the contributions of the other two types of edges. Hence we cannot avoid an additional parameter in our formulas, and the most convenient one is e_{33}. The following result is obtained in much the same way as Theorem 6, and we state it omitting the details.

Theorem 8. $M_2(B(h,i)) = 33h - 9 - 3i + e_{33}$. ■

From Theorems 2 and 8 it follows that for catacondensed benzenoids $e_{33} = h - 2 + B - S,$ a fact easily verified by direct computations.

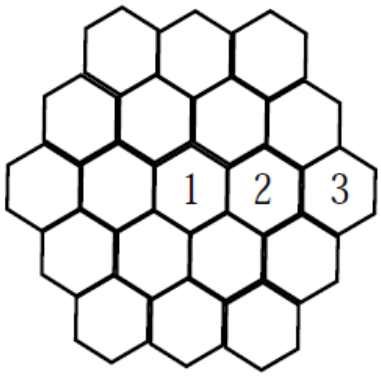

Figure 4: Hexagonal Benzenoid H_3 with 3 Layers of Hexagons.

Let us consider a benzenoid graph and connect the midpoints of all its peripheral hexagons in the way shown in Fig. 5. (We connect the midpoints by a segment across the shared edge) If the obtained figure is convex, such as the left one in Fig. 5, we say that the benzenoid graph is **convex**. Obviously, a benzenoid graph is convex if and only if $e_{33} = 0$. The only convex catacondensed benzenoid is the linear polyacene.

Figure 5: A Convex (left) and a Non-Convex (right) Benzenoid.

Corollary 9. Let K_h be a convex benzenoid on h hexagons. Then $M_2(K_h) \leq 33h - 9$. ■

It is clear that for establishing the lower bound we may restrict our attention on convex benzenoids with many internal edges. As in the case of M_1, by considering H_p we can see that for large enough p the value of $M_2(H_p)$ will be arbitrarily close to $27h$, again reflecting the fact that almost all edges are internal.

4. CONCLUDING REMARKS

We have considered the behavior of two Zagreb indices on catacondensed and pericondensed benzenoids. It has been shown that both indices are quite insensitive on the finer structural details. The first Zagreb index is unable to discriminate among

catacondensed benzenoids on the same number of hexagons and among the pericondensed benzenoids with the same number of internal vertices (on the same number of hexagons, of course). The second Zagreb index is mildly sensitive on the graph structure; its main source of variability comes from the deviation from convexity. Established lower and upper bounds are tight, but far from being sharp. Typically there are many benzenoids achieving the extremal values. The only exception seems to be the linear polyacene, reflecting the fact that it is the unique convex catacondensed benzenoid.

It would be straightforward to extend the presented analysis also to some other classes of graphs of chemical interest, such as the polyphenylenes. Another direction would be to examine some other invariants defined in terms of degree-dependent contributions of edges. We present a result of such type concerning the first Zagreb coindex.

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

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} [\delta(u) + \delta(v)],$$

where the summation is over all edges not in G. The quantity was introduced in a paper concerned with computing certain degree-weighted generalizations of Wiener polynomials [7]. The second Zagreb coindex is defined by the same modification of definition of the second Zagreb index. We refer the reader to [1] for some basic properties of Zagreb coindices. Among other results, there is a formula relating the first Zagreb index and the first Zagreb coindex of a graph G on n vertices and m edges,

$$\overline{M_1}(G) = 2\, m(n-1) - M_1(G).$$

By combining this formula with Theorem 1 we obtain the following result.

Corollary 10. Let B_h be a catacondensed benzenoid on h hexagons. Then

$$\overline{M_1}(B_h) = 4(10\, h^2 - 2\, h + 1).$$ ■

Similar results can be derived also for other classes of benzenoids, but we leave that to the reader.

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