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Zagreb Root-Indices of Graphs with Chemical Applications

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Abstract: Root-indices of graphs are mathematical tools that help us to understand complex systems, like molecules and networks, by capturing key structural information. In this study, we introduce two new root-indices, the first and the second Zagreb root-index, and we analyze their properties. We apply these indices to chemical structures like benzenoid molecules and octane isomers, showing that they sometimes provide better insights than traditional indices. We also compare the effectiveness of several root-indices with their standard versions, highlighting their ability to distinguish between different graph structures.

Keywords: the first Zagreb index; the second Zagreb index; root-indices; octane isomers; discrimination power

MSC: 05C09; 05C31; 05C07; 05C92; 92E10; 40A05

1. Introduction

Topological indices or topological descriptors are used in network theory to quantitatively describe the structure of the network topology [1,2]. This field began to develop with the introduction of the Wiener index, which is a fundamental concept in chemical graph theory, defined as the sum of the shortest path distances between all pairs of vertices in a graph, providing valuable insights into molecular structure and properties [3]. Later, several other topological indices were introduced, including the first Zagreb index and the second Zagreb index [4], which are degree-based.

For the indices mentioned above, corresponding graph polynomials can be considered: the first Zagreb polynomial and the second Zagreb polynomial (for example, see [5]).

The concept of utilizing the roots (zeros) of graph polynomials as structural descriptors has been a cornerstone in graph theory for decades, notably in the analysis of graph eigenvalues. On the other hand, it was shown [6] that if a polynomial Q fulfills certain conditions, then the modified polynomial $Q^* = 1 - Q$ has the unique positive root on the interval $(0, 1]$. This concept was firstly used for introducing a new measure of symmetry as the positive root of the modified orbit polynomial [6–8]. Recently, various modified distance-based graph polynomials have been defined, and their roots have been employed to establish new topological indices related to Wiener-like and Szeged-like indices, which are referred to as the root-indices [9,10].

In this paper, we continue with the previous work and therefore investigate two new root-indices: the first Zagreb root-index and the second Zagreb root-index. These root-indices overcome the limitations of traditional Zagreb indices by incorporating polynomial roots, offering improved discrimination power for chemical graph analysis. We firstly provide some analytical results and bounds related to the mentioned root-indices. Especially, we are interested in the behavior of these indices for basic graph families and for some chemical graphs.

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Citation: Tratnik, N.; Žigert Pleteršek, P. Zagreb Root-Indices of Graphs with Chemical Applications. *Mathematics* **2024**, *12*, 3871. https://doi.org/10.3390/math12233871

Academic Editor: Andrea Scozzari

Received: 13 November 2024
Revised: 6 December 2024
Accepted: 7 December 2024
Published: 9 December 2024

Next, we study correlations between the Zagreb root-indices (as well as eight other root-indices of graphs) and various molecular properties for all octane isomers. Additionally, we compute all possible correlation coefficients between the investigated molecular properties and the standard versions of the indices for octane isomers.

Finally, to assess the quality of the newly introduced measures, we evaluate the discrimination power of the Zagreb root-indices and compare their performance with both the standard versions of these indices and other root-indices.

2. Preliminaries

Let G be a connected graph with at least one edge. We denote by $\deg(u)$ the *degree* of vertex u.

Then, the *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$ are defined as follows [4]:

$$\begin{aligned} M_1(G) &= \sum_{uv\in E(G)} (\deg(u)+\deg(v)) = \sum_{u\in V(G)} \deg^2(u), \\ M_2(G) &= \sum_{uv\in E(G)} \deg(u)\deg(v). \end{aligned}$$

The *first Zagreb polynomial* of a graph G, denoted as $M_1(G,x)$, and the *second Zagreb polynomial* of G, denoted as $M_2(G,x)$, are defined in the following way:

$$\begin{aligned} M_1(G,x) &= \sum_{uv\in E(G)} x^{\deg(u)+\deg(v)}, \\ M_2(G,x) &= \sum_{uv\in E(G)} x^{\deg(u)\deg(v)}. \end{aligned}$$

Obviously, the first and the second Zagreb indices can be computed from the corresponding polynomials by evaluating their first derivatives at $x = 1$:

$$M_1(G) = M_1'(G,1), \qquad M_2(G) = M_2'(G,1).$$

Finally, we show an alternative way for writing the polynomials defined above. For a graph G and $k \geq 1$, we define the following sets of edges of G:

$$\begin{aligned} E_{1,k}(G) &= \{uv \in E(G) \mid \deg(u)+\deg(v) = k\}, \\ E_{2,k}(G) &= \{uv \in E(G) \mid \deg(u)\deg(v) = k\}. \end{aligned}$$

In addition, for every $k \geq 1$, we set

$$\begin{aligned} m_{1,k}(G) &= \left|E_{1,k}(G)\right|, \\ m_{2,k}(G) &= \left|E_{2,k}(G)\right|. \end{aligned}$$

It is straightforward to see that the following holds:

$$M_1(G,x) = \sum_{k\geq 2} m_{1,k}(G)\, x^k, \qquad M_2(G,x) = \sum_{k\geq 1} m_{2,k}(G)\, x^k.$$

The following numbers will be used in Section 4:

$$MM_1(G) = \max\{m_{1,k}(G) \mid k \geq 2\}, \qquad MM_2(G) = \max\{m_{2,k}(G) \mid k \geq 1\}.$$

3. Explicit Formulas for the First and the Second Zagreb Polynomials

Here, we state the explicit formulas for Zagreb polynomials for some families of graphs. It should be pointed out that the results are straightforward and some of them

were already stated in earlier papers. Hence, the proofs of the next two propositions are not included.

Proposition 1. *Let $n \geq 2$. For the complete graph K_n on n vertices and for the star S_n on $n+1$ vertices, the following holds:*

$$\begin{aligned} M_1(K_n, x) &= \tfrac{n(n-1)}{2} x^{2n-2}, & M_2(K_n, x) &= \tfrac{n(n-1)}{2} x^{(n-1)^2}, \\ M_1(S_n, x) &= n x^{n+1}, & M_2(S_n, x) &= n x^n. \end{aligned}$$

Proposition 2. *Let $n \geq 3$. For the cycle C_n on n vertices, the path P_n on n vertices, and the wheel W_n on $n+1$ vertices, the following holds:*

$$\begin{aligned} M_1(C_n, x) &= n x^4, & M_2(C_n, x) &= n x^4, \\ M_1(P_n, x) &= 2x^3 + (n-3)x^4, & M_2(P_n, x) &= 2x^2 + (n-3)x^4, \\ M_1(W_n, x) &= n x^{n+3} + n x^6, & M_2(W_n, x) &= n x^{3n} + n x^9. \end{aligned}$$

We now consider two infinite families of catacondensed benzenoid graphs and two families of phenylenes, which are all important molecular graphs. We firstly need several definitions.

A *benzenoid graph* is a simple 2-connected plane graph with all internal vertices of degree 3, all boundary vertices of degree 2 or 3, and all bounded faces hexagons (faces whose boundary is a 6-cycle). Note that in some literature, it is assumed that a benzenoid graph can be embedded into the regular hexagonal lattice [11].

A benzenoid graph is said to be *catacondensed* if it does not possess internal vertices. Otherwise, it is called *pericondensed*. Moreover, two hexagons of G are *adjacent* if they share exactly one edge.

Let G be a catacondensed benzenoid graph with at least two hexagons. If we add *quadrilaterals* (faces whose boundary is a 4-cycle) between all pairs of adjacent hexagons of G, the obtained graph G' is called a *phenylene*.

Let G be a catacondensed benzenoid graph or a phenylene, and let h be a hexagon of G. Hexagon h is called *terminal* if it is adjacent to exactly one other inner face of G, and it is called *branched* if it is adjacent to exactly three other inner faces of G. If h is adjacent to exactly two other inner faces, it has two vertices of degree two. Then, h is called *angular* if these two vertices are adjacent and *linear* it they are not adjacent. Moreover, a catacondensed benzenoid graph or a phenylene is called a *linear chain* if it does not contain angular or branched hexagons. The linear benzenoid chain with $n \geq 1$ hexagons will be denoted by BL_n, and the linear phenylene chain with $n \geq 2$ hexagons will be denoted by PL_n. Similarly, a catacondensed benzenoid graph or a phenylene is called an *angular chain* if it does not contain linear or branched hexagons. An angular benzenoid chain with $n \geq 1$ hexagons will be denoted by BA_n, and these graphs are also called fibonaccenes. Finally, an angular phenylene chain with $n \geq 2$ hexagons will be denoted by PA_n. See Figures 1 and 2.

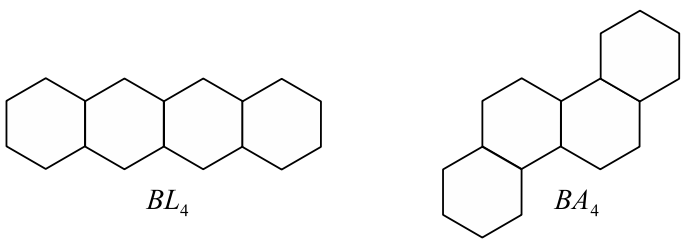
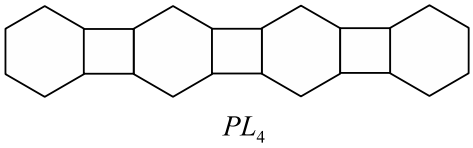
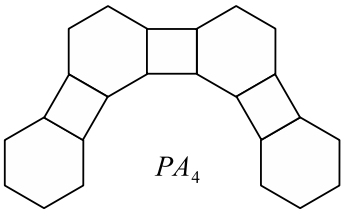


Figure 1. Linear benzenoid chain BL_4 and angular benzenoid chain BA_4.



PL_4



PA_4

Figure 2. Linear phenylene chain PL_4 and angular phenylene chain PA_4.

In the rest of this section, we calculate the first and the second Zagreb polynomial for linear and angular benzenoid chains and phenylene chains. In the proofs, we will need the following notation. For any $i, j \geq 1$ and any graph G, let

$$E^{i,j}(G) = \{uv \in E(G) \mid \{\deg(u), \deg(v)\} = \{i, j\}\}$$

and $m^{i,j}(G) = \left|E^{i,j}(G)\right|$.

Proposition 3. *Let $n \geq 1$. For benzenoid chains BL_n and BA_n, the following holds:*

$$\begin{aligned} M_1(BL_n, x) &= 6x^4 + (4n-4)x^5 + (n-1)x^6, \\ M_2(BL_n, x) &= 6x^4 + (4n-4)x^6 + (n-1)x^9, \\ M_1(BA_n, x) &= (n+4)x^4 + 2nx^5 + (2n-3)x^6, \\ M_2(BA_n, x) &= (n+4)x^4 + 2nx^6 + (2n-3)x^9. \end{aligned}$$

Proof. We can count the number of edges of particular degrees in BL_n and BA_n. Obviously,

$$\begin{aligned} m^{2,2}(BL_n) &= 6, & m^{2,2}(BA_n) &= n+4, \\ m^{2,3}(BL_n) &= 4n-4, & m^{2,3}(BA_n) &= 2n, \\ m^{3,3}(BL_n) &= n-1, & m^{3,3}(BA_n) &= 2n-3, \end{aligned}$$

and $m^{i,j}(BL_n) = m^{i,j}(BA_n) = 0$ for all other i, j. Consequently, we have

$$\begin{aligned} m_{1,4}(BL_n) = m_{2,4}(BL_n) &= 6, & m_{1,4}(BA_n) = m_{2,4}(BA_n) &= n+4, \\ m_{1,5}(BL_n) = m_{2,6}(BL_n) &= 4n-4, & m_{1,5}(BA_n) = m_{2,6}(BA_n) &= 2n, \\ m_{1,6}(BL_n) = m_{2,9}(BL_n) &= n-1, & m_{1,6}(BA_n) = m_{2,9}(BA_n) &= 2n-3. \end{aligned}$$

Note that $m_{1,k}(BL_n) = m_{2,k}(BL_n) = m_{1,k}(BA_n) = m_{2,k}(BA_n) = 0$ for all other k. Finally, we compute

$$\begin{aligned} M_1(BL_n, x) &= 6x^4 + (4n-4)x^5 + (n-1)x^6, \\ M_2(BL_n, x) &= 6x^4 + (4n-4)x^6 + (n-1)x^9, \\ M_1(BA_n, x) &= (n+4)x^4 + 2nx^5 + (2n-3)x^6, \\ M_2(BA_n, x) &= (n+4)x^4 + 2nx^6 + (2n-3)x^9. \end{aligned}$$

The proof is complete. □

Proposition 4. *Let $n \geq 2$. For phenylene chains PL_n and PA_n, the following holds:*

$$\begin{aligned} M_1(PL_n, x) &= 6x^4 + (4n-4)x^5 + (4n-4)x^6, \\ M_2(PL_n, x) &= 6x^4 + (4n-4)x^6 + (4n-4)x^9, \\ M_1(PA_n, x) &= (n+4)x^4 + 2nx^5 + (5n-6)x^6, \\ M_2(PA_n, x) &= (n+4)x^4 + 2nx^6 + (5n-6)x^9. \end{aligned}$$

Proof. Again, we can count the number of edges of particular degrees in PL_n and PA_n. Obviously,

$$\begin{aligned} m^{2,2}(PL_n) &= 6, & m^{2,2}(PA_n) &= n+4, \\ m^{2,3}(PL_n) &= 4n-4, & m^{2,3}(PA_n) &= 2n, \\ m^{3,3}(PL_n) &= 4n-4, & m^{3,3}(PA_n) &= 5n-6, \end{aligned}$$

and $m^{i,j}(PL_n) = m^{i,j}(PA_n) = 0$ for all other i, j. Consequently, we have

$$\begin{aligned} m_{1,4}(PL_n) = m_{2,4}(PL_n) &= 6, & m_{1,4}(PA_n) = m_{2,4}(PA_n) &= n+4, \\ m_{1,5}(PL_n) = m_{2,6}(PL_n) &= 4n-4, & m_{1,5}(PA_n) = m_{2,6}(PA_n) &= 2n, \\ m_{1,6}(PL_n) = m_{2,9}(PL_n) &= 4n-4, & m_{1,6}(PA_n) = m_{2,9}(PA_n) &= 5n-6. \end{aligned}$$

Note that $m_{1,k}(PL_n) = m_{2,k}(PL_n) = m_{1,k}(PA_n) = m_{2,k}(PA_n) = 0$ for all other k. Finally, we compute

$$\begin{aligned} M_1(PL_n, x) &= 6x^4 + (4n-4)x^5 + (4n-4)x^6, \\ M_2(PL_n, x) &= 6x^4 + (4n-4)x^6 + (4n-4)x^9, \\ M_1(PA_n, x) &= (n+4)x^4 + 2nx^5 + (5n-6)x^6, \\ M_2(PA_n, x) &= (n+4)x^4 + 2nx^6 + (5n-6)x^9, \end{aligned}$$

which completes the proof. □

4. Roots of Modified Degree-Based Polynomials

In this section, we investigate some newly defined polynomials. In particular, we introduce the following modified polynomials of a connected graph G:

$$\begin{aligned} M_1^*(G, x) &= 1 - M_1(G, x), \\ M_2^*(G, x) &= 1 - M_2(G, x). \end{aligned}$$

The motivation for studying these polynomials comes from a result used in [6], see also [9].

Lemma 1 ([6,9])**.** *Let $Q(x) = q_1x + q_2x^2 + \cdots + q_nx^n$ be a polynomial, $n \in \mathbb{N}$, $q_i \in [0, \infty)$ for all $i \in \{1, \ldots, n\}$, and $q_1 + q_2 + \cdots + q_n \geq 1$. Then, the polynomial $Q^*(x) = 1 - Q(x)$ has a unique positive root $\delta = \delta(Q^*(x))$ such that $\delta \in (0, 1]$. Moreover, $\delta = 1$ if and only if $q_1 + q_2 + \cdots + q_n = 1$.*

Obviously, if a connected graph has at least two vertices, then the polynomials M_1 and M_2 can be written as $q_1x + q_2x^2 + \cdots + q_nx^n$, where $n \in \mathbb{N}$, $q_i \in [0, \infty)$ for all $i \in \{1, \ldots, n\}$, and $q_1 + q_2 + \cdots + q_n \geq 1$.

According to Lemma 1, each of polynomials M_1^* and M_2^* has a unique positive root denoted as $\delta(M_1^*(G,x))$ and $\delta(M_2^*(G,x))$, respectively, which always lies within the interval $(0,1]$. This positive root serves as a topological index, referred to as a *root-index* [9]. In particular, $\delta(M_1^*)$ is the *first Zagreb root-index* and $\delta(M_2^*)$ is the *second Zagreb root-index*.

Proposition 5. *Let G be a connected graph with at least one edge and $i \in \{1,2\}$. Then, $\delta(M_i^*(G,x)) = 1$ if and only if G is isomorphic to K_2.*

Proof. Since

$$E(G) = \bigcup_{k\geq 2} E_{1,k}(G) = \bigcup_{k\geq 1} E_{2,k}(G),$$

we have

$$\sum_{k\geq 2} m_{1,k}(G) = |E(G)| \text{ and } \sum_{k\geq 1} m_{2,k}(G) = |E(G)|,$$

so the sum of all the coefficients in the polynomial $M_1(G,x)$ or $M_2(G,x)$ equals the number of edges of G. Based on Lemma 1 it holds that $\delta(M_i^*(G,x)) = 1$ if and only if the sum of all coefficients in polynomial $M_i(G,x)$ equals 1, where $i \in \{1,2\}$. Therefore, $\delta(M_i^*(G,x)) = 1$ if and only if G has only one edge. □

Next, we prove some lower bounds for both investigated root-indices. Note that we are able to obtain better lower bounds as for Szeged- and Wiener-like root-indices [9,10].

Theorem 1. *Let G be a connected graph with at least one edge. Then,*

$$\begin{aligned}
\delta(M_1^*(G,x)) &> \frac{-1+\sqrt{4MM_1(G)+1}}{2MM_1(G)} > \frac{1}{MM_1(G)+1}, \\
\delta(M_2^*(G,x)) &> \frac{-1+\sqrt{4MM_2(G)+1}}{2MM_2(G)} > \frac{1}{MM_2(G)+1}.
\end{aligned}$$

Proof. Let $\delta = \delta(M_1^*(G,x))$. Obviously, the result holds trivially if $\delta = 1$, so in the following, suppose that $\delta < 1$. We consider

$$M_1(G,\delta) = \sum_{k\geq 2} m_{1,k}(G)\delta^k,$$

where $m_{1,k}(G)$ is the number of edges $uv \in E(G)$ for which $\deg(u) + \deg(v) = k$. We start with

$$M_1(G,\delta) = \sum_{k\geq 2} m_{1,k}(G)\delta^k < \sum_{k\geq 2} MM_1(G)\delta^k = MM_1(G)\sum_{k=2}^{\infty}\delta^k = MM_1(G)\frac{\delta^2}{1-\delta}.$$

Consequently, it holds

$$\sum_{k\geq 2} m_{1,k}(G)\delta^k < MM_1(G)\frac{\delta^2}{1-\delta}. \tag{1}$$

However, it obviously holds that

$$M_1^*(G,\delta) = 0,$$

so from $M_1^*(G,\delta) = 1 - M_1(G,\delta)$ we also obtain

$$M_1(G,\delta) = \sum_{k\geq 2} m_{1,k}(G)\delta^k = 1. \tag{2}$$

Finally, Equations (1) and (2) imply

$$1 < MM_1(G)\frac{\delta^2}{1-\delta},$$

which gives

$$MM_1(G)\delta^2 + \delta - 1 > 0$$

and since $MM_1(G) > 0$, $\delta \in (0,1)$, we consequently have

$$\delta > \frac{-1 + \sqrt{4MM_1(G) + 1}}{2MM_1(G)}.$$

Through straightforward calculation we can show that

$$\frac{-1 + \sqrt{4MM_1(G) + 1}}{2MM_1(G)} > \frac{1}{MM_1(G) + 1},$$

which completes the first part of the proof.

For the second part, suppose that $\delta = \delta(M_2^*(G,x))$. Again, the result holds trivially if $\delta = 1$, so in the following, assume that $\delta < 1$. Therefore, G has more than two vertices based on Proposition 5. Consequently, $m_{2,1}(G) = 0$, and the polynomial $M_2(G,x)$ can be written as follows:

$$M_2(G,x) = \sum_{k\geq 2} m_{2,k}(G)x^k.$$

By using the same arguments as before, we obtain

$$\delta > \frac{-1 + \sqrt{4MM_2(G) + 1}}{2MM_2(G)} > \frac{1}{MM_2(G) + 1},$$

so the proof is complete. □

As an example, we apply the previous theorem on linear benzenoid chains. It is easy to observe that for $n \geq 3$,

$$MM_1(BL_n) = MM_2(BL_n) = 4n - 4,$$

which implies that

$$\delta(M_1^*(BL_n,x)) > \frac{-1 + \sqrt{16n - 15}}{8n - 8} \text{ and } \delta(M_2^*(BL_n,x)) > \frac{-1 + \sqrt{16n - 15}}{8n - 8}.$$

For instance, if $n = 4$, we can compute the roots

$$\delta(M_1^*(BL_n,x)) \approx 0.5253 \text{ and } \delta(M_2^*(BL_n,x)) \approx 0.5628,$$

while on the other hand, the lower bound equals

$$\frac{-1 + \sqrt{16 \times 4 - 15}}{8 \times 4 - 8} \approx 0.25.$$

In the rest of this section, we consider the root-indices of basic graph families and investigate their behavior for large n. We firstly recall the following lemma from [10].

Lemma 2 ([10]). *For any $n \geq 1$, let $Q_n(x) = q_{n,1}x + q_{n,2}x^2 + \cdots + q_{n,m_n}x^{m_n}$ be a polynomial that satisfies the conditions of Lemma 1. Moreover, suppose that there exists a constant $k \geq 1$ and a polynomial p with degree at least one such that for every $n \geq 1$, it holds that $q_{n,k} = p(n)$. If $c_n = \delta(Q_n^*(x))$ for all $n \geq 1$, then the sequence (c_n) converges to 0.*

By using the stated result, we obtain the next proposition.

Proposition 6. *For any $n \geq 3$, let $a_n = \delta(M_1^*(C_n, x))$, $b_n = \delta(M_2^*(C_n, x))$, $c_n = \delta(M_1^*(P_n, x))$, $d_n = \delta(M_2^*(P_n, x))$, $e_n = \delta(M_1^*(W_n, x))$, and $f_n = \delta(M_2^*(W_n, x))$. Then,*

$$\lim_{n\to\infty} a_n = \lim_{n\to\infty} b_n = \lim_{n\to\infty} c_n = \lim_{n\to\infty} d_n = \lim_{n\to\infty} e_n = \lim_{n\to\infty} f_n = 0.$$

Proof. We already know that for $n \geq 3$, it holds that

$$M_1(C_n, x) = nx^4.$$

Let $k = 4$. Then, the coefficient before x^k equals n, which is a polynomial with degree at least 1. Based on Lemma 2, we have

$$\lim_{n\to\infty} a_n = 0.$$

In a similar way, we can show that all the other sequences also converge to 0. □

Analogously, we can describe the behavior of Zagreb root-indices of benzenoid chains and phenylene chains.

Proposition 7. *For any $n \geq 2$, we denote $a_n = \delta(M_1^*(BL_n, x))$, $b_n = \delta(M_2^*(BL_n, x))$, $c_n = \delta(M_1^*(BA_n, x))$, $d_n = \delta(M_2^*(BA_n, x))$, $e_n = \delta(M_1^*(PL_n, x))$, $f_n = \delta(M_2^*(PL_n, x))$, $g_n = \delta(M_1^*(PA_n, x))$, and $h_n = \delta(M_2^*(PA_n, x))$. Then,*

$$\lim_{n\to\infty} a_n = \lim_{n\to\infty} b_n = \lim_{n\to\infty} c_n = \lim_{n\to\infty} d_n = \lim_{n\to\infty} e_n = \lim_{n\to\infty} f_n = \lim_{n\to\infty} g_n = \lim_{n\to\infty} h_n = 0.$$

On the other hand, based on Proposition 1 we immediately obtain the following result.

Proposition 8. *Let $n \geq 2$. For the complete graph K_n on n vertices and for the star S_n on $n+1$ vertices, the following holds:*

$$\begin{aligned} \delta(M_1^*(K_n, x)) &= \left(\tfrac{2}{n(n-1)}\right)^{\frac{1}{2n-2}}, & \delta(M_2^*(K_n, x)) &= \left(\tfrac{2}{n(n-1)}\right)^{\frac{1}{(n-1)^2}}, \\ \delta(M_1^*(S_n, x)) &= \left(\tfrac{1}{n}\right)^{\frac{1}{n+1}}, & \delta(M_2^*(S_n, x)) &= \left(\tfrac{1}{n}\right)^{\frac{1}{n}}. \end{aligned}$$

Consequently, this gives us the next proposition.

Proposition 9. *For any $n \geq 2$, let $a_n = \delta(M_1^*(K_n, x))$, $b_n = \delta(M_2^*(K_n, x))$, $c_n = \delta(M_1^*(S_n, x))$, and $d_n = \delta(M_2^*(S_n, x))$. Then,*

$$\lim_{n\to\infty} a_n = \lim_{n\to\infty} b_n = \lim_{n\to\infty} c_n = \lim_{n\to\infty} d_n = 1.$$

Proof. Since

$$a_n = \left(\frac{2}{n(n-1)}\right)^{\frac{1}{2n-2}},$$

for any $n \geq 2$, we calculate the limit

$$\lim_{x\to\infty} \left(\frac{2}{x(x-1)}\right)^{\frac{1}{2x-2}} = e^{\lim_{x\to\infty} \frac{1}{2x-2} \ln\left(\frac{2}{x(x-1)}\right)}$$

using L'Hospital's rule. We obtain

$$\lim_{x\to\infty} \frac{1}{2x-2} \ln\left(\frac{2}{x(x-1)}\right) = \lim_{x\to\infty} \left(\frac{1}{2} \cdot \frac{x(x-1)}{2} \cdot \frac{-2(2x-1)}{x^2(x-1)^2}\right) = 0,$$

so

$$\lim_{n\to\infty} a_n = e^0 = 1.$$

In a similar way, one can calculate the remaining three limits. □

5. Applications of Root-Indices to Octane Isomers

In this section, we compare the first Zagreb root-index and the second Zagreb root-index, as well as eight other root-indices of graphs with 15 different molecular properties for all 18 octane isomers. The molecular properties were obtained from the dataset proposed by the International Academy of Mathematical Chemistry (downloaded in 2017 from the IAMC website). We used our own programming code written in SageMath to calculate 10 root-indices of graphs. In addition to both Zagreb root-indices, we also investigated the following indices: the Wiener root-index $\delta(H^*)$, the edge-Wiener root-index $\delta(H_e^*)$, the Gutman root-index $\delta(Gut^*)$, the Schultz root-index $\delta(Sc^*)$, the Szeged root-index $\delta(Sz^*)$, the weighted-product Szeged root-index $\delta(wSz_1^*)$, the weighted-plus Szeged root-index $\delta(wSz_2^*)$, and the Mostar root-index $\delta(Mo^*)$. For the definitions and more details on the mentioned root-indices, see [9,10].

On the other hand, we consider the following molecular properties:

- boling point (BP),
- heat capacity at T constant (CT),
- heat capacity at P constant (CP),
- entropy (S),
- density (DENS),
- enthalpy of vaporization (HVAP),
- standard enthalpy of vaporization (DVAP),
- enthalpy of formation (HFORM),
- standard enthalpy of formation (DFORM),
- motor octane number (MON),
- molar refraction (MR),
- acentric factor (ACF),
- total surface area (TSA),
- octanol-water partition coefficient (LogP),
- molar volume (MV).

We calculated all possible correlation coefficients between the investigated molecular properties and root-indices for octane isomers by using RStudio. The results are gathered in Figure 3. We can observe that both newly introduced Zagreb root-indices have good correlation with the boiling point ($R = -0.82$ and $R = -0.87$). In fact, those are the best results for this property among all considered root-indices. Note that the first Zagreb root-index has excellent correlations ($R > 0.9$) with four molecular properties: entropy, enthalpy of vaporization, standard enthalpy of vaporization, and acentric factor. Similarly, the second Zagreb root-index has very good correlations with the enthalpy of vaporization and enthalpy of formation.

Among all root-indices, the best correlation is found between the Wiener root-index and the acentric factor ($R = 0.99$). Several very high correlations can be seen also for the following properties: entropy, enthalpy of vaporization, standard enthalpy of vaporization, acentric factor. These correlations are achieved by distance-based root-indices except for the Mostar index.

Next, we investigate the efficiency of root-indices with regard to the standard versions of them. Therefore, we also calculate all possible correlation coefficients between the investigated molecular properties and standard indices for octane isomers. The results are gathered in Figure 4.

We observe that in general, the performance is quite similar, but several cases show that the root-indices outperform their standard counterparts. To facilitate the comparison of the two tables shown in Figures 3 and 4, we also present a table showing the differences

in absolute values of the correlation coefficients; see Figure 5. We notice that there are many cells in the red spectrum, which indicates that in these cases, a root-index surpasses the standard index.

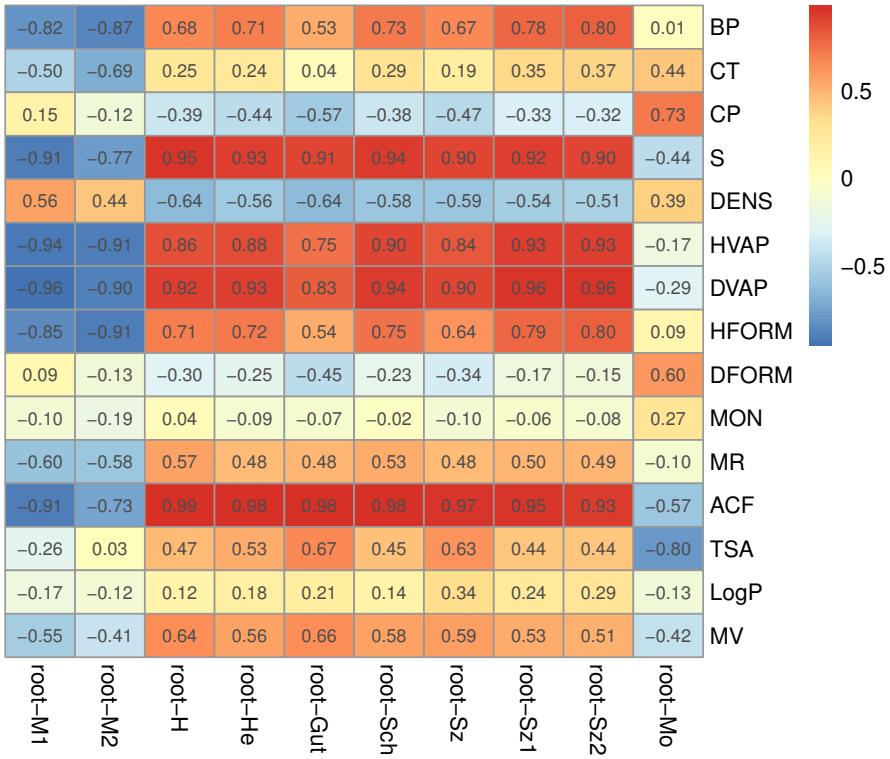


Figure 3. A heatmap of correlation coefficients between molecular properties and root-indices for the set of 18 octane isomers. For example, the notation "root-M1" represents the first Zagreb root-index.

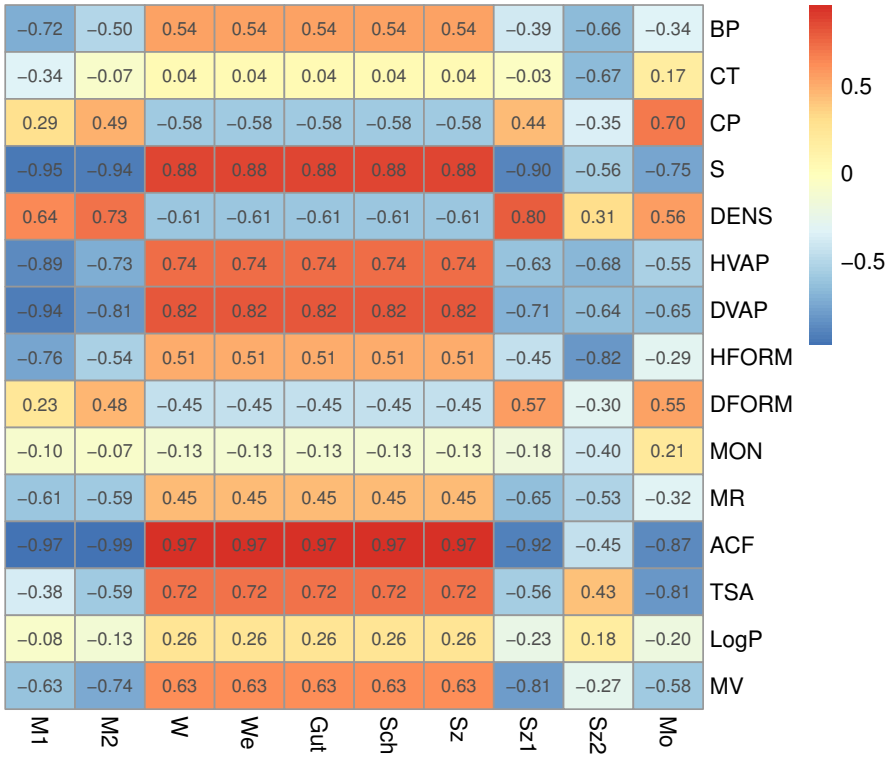


Figure 4. A heatmap of correlation coefficients between molecular properties and standard indices for the set of 18 octane isomers.

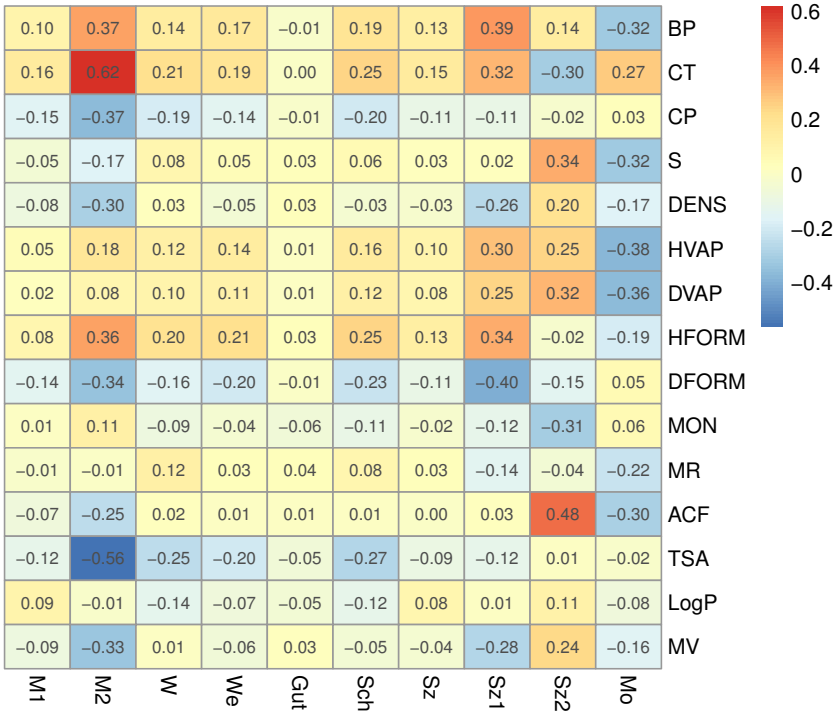


Figure 5. Heatmap of differences in absolute values for the data in Figures 3 and 4.

6. Discrimination Power

In this section, we investigate the discrimination power of root-indices and compare the results with standard indices. More precisely, we consider the discrimination (also called sensitivity), which is the concept introduced in [12]. Let $\mathcal{C}$ be any finite family of pairwise non-isomorphic graphs, and TI is a topological index. Moreover, let $\mathcal{N}$ be the set of all graphs from $\mathcal{C}$ that cannot be discriminated by topological index TI. In addition, let $N = |\mathcal{N}|$. The *discrimination* D of a topological index TI is defined as

$$D(TI) = \frac{|\mathcal{C}| - N}{|\mathcal{C}|}.$$

Furthermore, by N_r and T_r we denote the sets of all connected graphs and all trees on r vertices, respectively. For families N_r, where $r \in \{5, 6, 7, 8\}$, and T_r, where $r \in \{8, \ldots, 16\}$, we have computed N and discrimination for the first Zagreb root-index, the second Zagreb root-index, and both standard versions of them. The results are presented in Table 1.

We observe that the root-indices have much better discrimination power than their standard versions. For example, the first Zagreb root-index can discriminate more than 70% of trees on nine vertices, but the corresponding standard index can distinguish less than 11% of these trees. However, we observe that also for root-indices, the strength of the discrimination decreases rapidly as the number of vertices increases.

It is also interesting to compare these results with the Szeged-like and Wiener-like root-indices of graphs, which were considered in [9,10]. For example, the weighted-product Szeged root-index and the weighted-sum Szeged-root index have much higher discrimination than the Zagreb root-indices. On the other hand, the Szeged root-index and the Mostar root-index have more or less the same discrimination power on families of trees, while the former performs much better on the families of all connected graphs compared to the Zagreb root-indices. A comparison with the Wiener-like root-indices shows that they discriminate graphs much better than the Zagreb root-indices on families of trees, while on the families of general connected graphs, the Zagreb root-indices have slightly better discrimination than the Wiener-like root-indices, with the exception of the Gutman root-index.

Table 1. Discrimination for Zagreb root-indices and standard indices in different families of graphs and trees.

		$\delta(M_1^*)$		$\delta(M_2^*)$		M_1		M_2	
Family	**No. of Graphs**	N	D	N	D	N	D	N	D
all connected graphs									
N_5	21	0	1.0000	0	1.0000	10	0.5238	0	1.0000
N_6	112	22	0.8036	22	0.8036	98	0.1250	37	0.6696
N_7	853	441	0.4830	408	0.5217	841	0.0141	750	0.1208
N_8	11,117	8896	0.1998	8515	0.2341	11,103	0.0013	10,996	0.0109
all tree structures									
T_8	23	4	0.8261	4	0.8261	19	0.1739	12	0.4783
T_9	47	14	0.7021	14	0.7021	42	0.1064	37	0.2128
T_{10}	106	48	0.5472	45	0.5755	100	0.0566	93	0.1226
T_{11}	235	137	0.4170	131	0.4426	230	0.0213	222	0.0553
T_{12}	551	387	0.2976	376	0.3176	545	0.0109	539	0.0218
T_{13}	1301	1015	0.2198	995	0.2352	1294	0.0054	1290	0.0085
T_{14}	3159	2669	0.1551	2642	0.1637	3153	0.0019	3143	0.0051
T_{15}	7741	6923	0.1057	6853	0.1147	7735	0.0008	7725	0.0021
T_{16}	19,320	17,963	0.0702	17,832	0.0770	19,313	0.0004	19,306	0.0007

7. Conclusions

In this study, we introduced two novel root-indices: the first Zagreb root-index and the second Zagreb root-index. We established lower bounds for these root-indices and examined their behavior across basic families of graphs. Our analysis reveals that, for the majority of these families, the sequence of root-indices converges to zero as the number of vertices increases, with the exception of complete graphs and stars. Additionally, we presented the results for four significant classes of chemical graphs, which are subfamilies of benzenoid and phenylene chains.

We then explored the chemical applications of the Zagreb root-indices, Szeged-like root-indices, and Wiener-like root-indices concerning various properties of octane isomers. We computed correlation coefficients between the molecular properties and both the newly introduced root-indices and their standard counterparts. Our findings indicate a generally comparable performance between the two sets of indices; however, there are instances where a root-index demonstrates superior predictive capability. Notably, the correlation coefficient between the second Zagreb root-index and heat capacity at a constant temperature is -0.69, in contrast to -0.07 for the second Zagreb index.

Regarding the discrimination power, our results suggest that the Zagreb root-indices are more effective at distinguishing between graphs than standard indices. However, their performance is in general still weaker than that of other previously introduced root-indices.

For future research, it would be valuable to investigate new bounds and analytical results for the newly introduced root-indices, as well as to explore additional chemical applications.

Author Contributions: N.T. and P.Ž.P. contributed equally to this work. Conceptualization, N.T. and P.Ž.P.; methodology, N.T. and P.Ž.P.; software, N.T. and P.Ž.P.; validation, N.T. and P.Ž.P.; formal analysis, N.T. and P.Ž.P.; investigation, N.T. and P.Ž.P.; resources, N.T. and P.Ž.P.; data curation, N.T. and P.Ž.P.; writing—original draft preparation, N.T. and P.Ž.P.; writing—review and editing, N.T. and P.Ž.P.; visualization, N.T. and P.Ž.P.; supervision, N.T. and P.Ž.P.; project administration, N.T. and P.Ž.P.; funding acquisition, N.T. and P.Ž.P. All authors have read and agreed to the published version of the manuscript.

Funding: The authors acknowledge financial support from the Slovenian Research and Innovation Agency: research programme no. P1-0297 (Niko Tratnik, Petra Žigert Pleteršek), project no. N1-0285 (Niko Tratnik), and project no. L7-4494 (Petra Žigert Pleteršek).

Data Availability Statement: The data supporting the conclusions (values of root-indices, standard indices, and molecular properties for octane isomers) will be made available by the authors upon request.

Conflicts of Interest: The authors declare no conflicts of interest.

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