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COMPUTATION OF SOME DEGREE-BASED TOPOLOGICAL INDICES OF [n]CIRCULENES ACCORDING TO THE SIZE OF THEIR CENTRAL POLYGON

Z. RAJABINEJAD[1], S. MOHAMMADIAN SEMNANI[1*], §

Abstract. In this paper, several degree-based topological indices are computed for the family of [n]circulenes, a class of polycyclic hydrocarbons, using the M-polynomial method, which eliminates edge counting. Closed-form formulas depending only on the central polygon size n are derived for indices including the First and Second Zagreb, Modified Zagreb, Harmonic, Symmetric Division Degree, Inverse Sum, and Sigma indices. Numerical and graphical analyses for $n = 3$ to 10 reveal increasing trends, reflecting growing structural complexity. Additionally, an asymptotic analysis explores the behavior of these indices as $n \to \infty$. These results offer a unified and scalable computational framework that fills a theoretical gap and aids quantitative structure–property relationship modeling of complex polycyclic systems.

Keywords: Graph theory, [n]Circulenes., M-polynomial, Degree-based topological index.

AMS Subject Classification: 05C31, 05C92, 05C09, 05C30, 05C90.

1. Introduction

The class of [n]circulenes is a special family of polycyclic aromatic hydrocarbons constructed by a central n-sided polygon fused with n benzene rings. Due to their high symmetry and well-defined structural patterns, these molecules have attracted considerable attention in theoretical and applied chemistry [1, 2, 3]. Their geometry varies with n: for $3 \leq n \leq 5$, the structure is bowl-shaped with positive curvature; for $n = 6$, it is planar; for $7 \leq n \leq 16$, it adopts a saddle-shaped geometry with negative curvature; and for $n \geq 17$, they form helical structures, see Figure 1.

For analyzing the structure of these molecules, graph modeling is very effective, with atoms represented as vertices and chemical bonds as edges. From a chemical perspective, [n]circulenes exhibit unique aromatic stability and electronic and optical properties,

[1] Department of Mathematics, Faculty of Mathematics, Statistics and Computer Science, Semnan University, Semnan, Iran
e-mail: zohreh_rajabinejad@semnan.ac.ir; ORCID no. 0009-0008-0379-0120.
[1] Department of Mathematics, Faculty of Mathematics, Statistics and Computer Science, Semnan University, Semnan, Iran
e-mail: s_mohammadian@semnan.ac.ir; ORCID no. 0000-0001-6755-4911.
[*] Corresponding author
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making them valuable in fields such as nanophotonics, organic semiconductors, hydrogen storage, and molecular sensors [4, 5]. Their spatial symmetry and chirality also make them attractive candidates for stereochemical studies and the design of chiral materials. These molecules can be modeled as molecular graphs with high symmetry, enabling the systematic computation of topological indices. Chemical graph theory provides a mathematical framework connecting graph theory and chemistry by representing molecules as graphs [6, 7]. This approach facilitates the extraction of topological and structural features of molecules using graph-theoretic techniques. Vertex degree and atomic distances are among key features used to estimate physicochemical properties such as boiling points [8]. Among the important tools in this domain are topological polynomials, such as the M-polynomial and the SMP-polynomial, which enable the symbolic computation of degree-based topological indices [9, 10].

In this paper, our primary objective is to derive closed-form expressions for degree-based topological indices of $[n]$circulene graphs using the M-polynomial, providing an exact and efficient method without the need for manual edge counting or partitioning.

Topological indices (TIs) are numerical descriptors that encode important structural properties of molecular graphs such as size, branching, and connectivity. Degree-based indices, including First Zagreb (FZ), Second Zagreb (SZ), Modified Zagreb (MZ), Harmonic (H), Symmetric Division Deg (SDD), Inverse Sum (I), Sigma (σ), and others, have been widely used in QSPR/QSAR modeling to predict physicochemical, biological, and pharmaceutical properties of molecules [10, 11, 12]. Precise definitions and formulas for these indices are provided in Section 2.

Topological polynomials serve as essential tools in graph theory, facilitating the computation of various TIs. Among these, the Hosoya polynomial is fundamental as it encodes the vertex distance information of a graph, which enables the extraction of distance-based indices used in chemical graph analysis [13]. Another important polynomial is the SMP-polynomial, introduced by Knor and Tratnik, which has proven highly effective for calculating indices such as the Szeged, PI, and Mostar indices [14, 15]. Moreover, the M-polynomial, introduced by Deutsch and Klavžar in 2015, provides a powerful and unified framework for computing degree-based TIs. It is defined as [16, 17]:

$$M(G;x,y)=\sum_{\delta\leq i\leq j\leq\Delta} m_{ij}(G)x^iy^j,$$

Where δ and Δ represent the minimum and maximum vertex degrees of the graph G, respectively, and $m_{ij}(G)$ denotes the number of edges whose endpoints have degrees i and j. The M-polynomial not only streamlines the computation of numerous degree-based indices but also aids in predicting chemical properties of complex molecules, including nanostructures and polycyclic aromatic hydrocarbons, which are of significant interest in chemical graph theory and nanotechnology [18, 19, 20]. Building on this, the NM-polynomial, which focuses on sums of neighbor degrees, has emerged as another valuable tool in this domain [21]. Together, these polynomials form the fundamental framework of modern TI calculations, offering both theoretical insights and practical computational advantages.

In recent years, significant progress has been made in computing degree-based TIs through the use of polynomial-based techniques. In 2021, an effective method for computing the σ index and other degree-based indices via the M-polynomial was proposed by Rajpoot and Selvaganesh, and applied to carbon nanotube structures $\mathrm{HC_5C_7}[p,q]$ and $\mathrm{VC_5C_7}[p,q]$ [22]. In 2023, Chaudhry et al. computed M-polynomials and degree-based

indices of tadpole graphs, demonstrating the efficiency of this approach [23]. More recently, in 2024, the degree-based indices of Dandelion graphs and their line graphs were investigated using M-polynomial techniques by Nagesh et al. [24]. In 2025, degree-based indices of fractional coronene graphs were determined using polynomial methods by Zhu et al., offering new insights into the topological characteristics of circulene structures [25]. Although distance-based indices of $[n]$circulenes graphs have been derived using the SMP-polynomial by Rajabinejad and Mohammadian Semnani [26], to the best of the authors' knowledge, closed formulas for degree-based TIs of $[n]$circulenes based on the M-polynomial have not yet been reported in the literature.

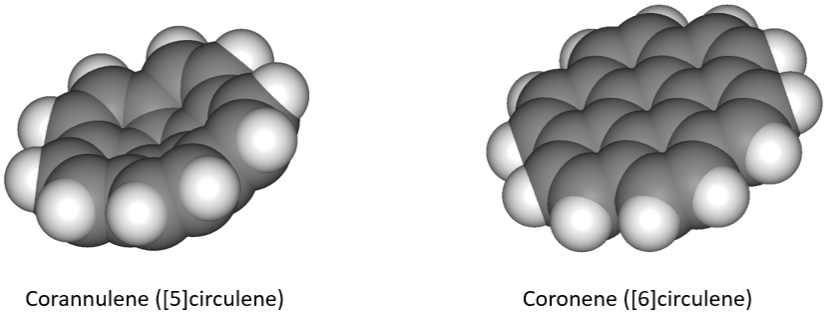

FIGURE 1. Three-dimensional space-filling representations of [5]circulene and [6]circulene molecules. The structures illustrate the bowl-shaped geometry of [5]circulene and the nearly planar structure of [6]circulene.

2. Methodology

Initially, the concept of $[n]$circulenes and their significance in theoretical and computational chemistry are reviewed. These polycyclic structures are of particular interest due to their unique electronic and topological properties, making them suitable for mathematical modeling.

The core of our approach lies in deriving explicit analytical formulas for degree-based TIs of $[n]$circulenes. This is achieved by analyzing the geometric and topological features of these cyclic structures, particularly the size of the central polygon and the connectivity patterns of adjacent rings and vertices. To this end, the edges of the graph are categorized based on the degrees of their end vertices, which enables the construction of the M-polynomial.

After establishing the M-polynomial, various degree-based TIs such as the FZ, SZ, MZ, H, SDD, I, and σ are computed by applying differential and integral operators to $M(G;x,y)$. This operator-based framework eliminates the need for manual edge enumeration and provides a systematic way of computing these indices.

The operators used in this computation are defined as follows:

$$D_x = x\frac{\partial}{\partial x}, \quad D_y = y\frac{\partial}{\partial y}, \quad JM(x,y) = M(x,x),$$
$$S_x = \int_0^x \frac{M(t,y)}{t}dt, \quad S_y = \int_0^y \frac{M(x,t)}{t}dt,$$

where D_x and D_y denote partial differential operators, and S_x and S_y represent integral operators. This operator-based method not only simplifies the computational process but

also enables the explicit derivation of closed-formulas for various indices as functions of the parameter n, which characterizes the size of the central polygon in the $[n]$circulene structure. To better understand the methods for calculating TIs, an overview of the aforementioned indices is first provided.

Gutman and Trinajstić introduced the FZ Index, which is defined as [27]:

$$FZ = \sum_{uv \in E(G)} (d_u + d_v),$$

where d_u and d_v denote the degrees of the vertices u and v, respectively. SZ index is given by [28]:

$$SZ = \sum_{uv \in E(G)} d_u d_v.$$

The MZ Index, defined as the sum of the reciprocals of the products of degrees of adjacent vertices, is given by [29]:

$$MZ = \sum_{uv \in E(G)} \frac{1}{d_u d_v}.$$

H serving as a counterpart to the Randić index, it is defined by [30]:

$$H = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

The SDD index was introduced in 2010 by Vukičević and Gašperov as one of the discrete Adriatic indices. It characterizes molecular structures more accurately by using the ratio of degrees of adjacent vertices, and is defined as follows [31]:

$$SDD(G) = \sum_{uv \in E(G)} \left(\frac{d_u}{d_v} + \frac{d_v}{d_u} \right) = \sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u d_v},$$

where G is a molecular graph, $E(G)$ is its edge set, and d_u, d_v are the degrees of the vertices u and v, respectively.

The inverse sum index is defined by [32]:

$$I = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}$$

The σ index, measuring the squared difference of degrees of adjacent vertices, is defined as [33]:

$$\sigma = \sum_{uv \in E(G)} (d_u - d_v)^2.$$

In the subsequent sections, the accuracy and efficiency of the proposed method are evaluated through numerical computations, graphical representations, and asymptotic analysis as $n \to \infty$. Finally, the implications of the results are discussed within the framework of chemical graph theory, and a concluding summary is presented.

3. Main result

Let $G = \mathcal{C}_n$ be the molecular graph of $[n]$circulenes, where n denotes the size of the central polygon. Here, $p = 4n$ and $q = 5n$ represent the number of vertices and edges of $\mathcal{C}_n$, respectively. See the molecular graph of $[n]$circulenes in Figure 2. Table 1 provides detailed information about the number of vertices and edges, the size of the central polygon, the classification of edges based on vertex degrees, and the frequency of each edge type. This

study focuses on degree-based TIs, which are widely used to predict physicochemical, biological, and pharmaceutical properties of molecules in QSPR/QSAR models [10, 11, 12]. The degree-based TIs derived from the M-polynomial are summarized in Table 2.

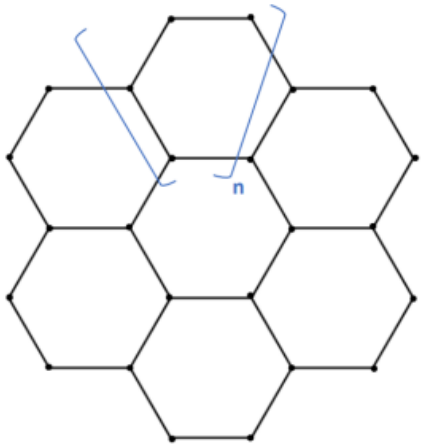

FIGURE 2. The base graph of the $[n]$circulenes for $n \geq 4$.

TABLE 1. Edge classification of the $[n]$circulenes graph.

Edges types	m_{22}	m_{23}	m_{33}	q	p
Number	n	$2n$	$2n$	$5n$	$4n$

TABLE 2. Degree-based Topological indices derived from the M-polynomial.

Topological index	Derivative from $M = M(G; x, y)$
First Zagreb	$(D_x + D_y)M\|_{x=y=1}$
Second Zagreb	$(D_x D_y)M\|_{x=y=1}$
Modified Zagreb	$(S_x S_y)M\|_{x=y=1}$
Harmonic	$2S_x JM\|_{x=y=1}$
Symmetric Division Deg	$(D_x S_y + D_y S_x)M\|_{x=y=1}$
Inverse sum	$(S_x J D_x D_y)M\|_{x=1}$
Sigma	$(D_x^2 + D_y^2 - 2D_x D_y)M\|_{x=y=1}$

Theorem 3.1. *Consider $\mathcal{C}_n$ to be the molecular graph of $[n]$circulenes, where $n \geq 3$. Then, the M-polynomial of $\mathcal{C}_n$ is given by:*

$$M(\mathcal{C}_n; x, y) = nx^2y^2 + 2nx^2y^3 + 2nx^3y^3.$$

Proof. Using Table 1, the M-polynomial of $\mathcal{C}_n$ is calculated as follows:

$$\begin{aligned} M(\mathcal{C}_n; x, y) &= \sum_{2 \leq i \leq j \leq 3} m_{ij}(\mathcal{C}_n) x^i y^j \\ &= \sum_{2 \leq 2} m_{22}(\mathcal{C}_n) x^2y^2 + \sum_{2 \leq 3} m_{23}(\mathcal{C}_n) x^2y^3 + \sum_{3 \leq 3} m_{33}(\mathcal{C}_n) x^3y^3 \\ &= nx^2y^2 + 2nx^2y^3 + 2nx^3y^3 \end{aligned}$$

□

Proposition 3.1. *Let $\mathcal{C}_n$ be the graph of $[n]$circulenes, where $n \geq 3$. Then, the following hold:*

(i) $FZ(\mathcal{C}_n) = 26n$,
(ii) $SZ(\mathcal{C}_n) = 34n$,
(iii) $SDD(\mathcal{C}_n) = \frac{31}{3}n$,
(iv) $MZ(\mathcal{C}_n) = \frac{29}{36}n$,
(v) $H(\mathcal{C}_n) = \frac{59}{30}n$,
(vi) $I(\mathcal{C}_n) = \frac{32}{5}n$,
(vii) $\sigma(\mathcal{C}_n) = 2n$.

Proof. Let $M(\mathcal{C}_n; x, y) = nx^2y^2 + 2nx^2y^3 + 2nx^3y^3$. The following results are obtained by applying the operators on the M-polynomial:

$$\begin{aligned}
D_xM(\mathcal{C}_n; x, y) &= 2nx^2y^2 + 4nx^2y^3 + 6nx^3y^3,\\
D_yM(\mathcal{C}_n; x, y) &= 2nx^2y^2 + 6nx^2y^3 + 6nx^3y^3,\\
D_x^2M(\mathcal{C}_n; x, y) &= 4nx^2y^2 + 8nx^2y^3 + 18nx^3y^3,\\
D_y^2M(\mathcal{C}_n; x, y) &= 4nx^2y^2 + 18nx^2y^3 + 18nx^3y^3,\\
D_xD_yM(\mathcal{C}_n; x, y) &= 4nx^2y^2 + 12nx^2y^3 + 18nx^3y^3,\\
S_xM(\mathcal{C}_n; x, y) &= \frac{n}{2}x^2y^2 + nx^2y^3 + \frac{2n}{3}x^3y^3,\\
S_yM(\mathcal{C}_n; x, y) &= \frac{n}{2}x^2y^2 + \frac{2n}{3}x^2y^3 + \frac{2n}{3}x^3y^3,\\
S_xS_yM(\mathcal{C}_n; x, y) &= \frac{n}{4}x^2y^2 + \frac{n}{3}x^2y^3 + \frac{2n}{9}x^3y^3,\\
D_xS_yM(\mathcal{C}_n; x, y) &= nx^2y^2 + \frac{4n}{3}x^2y^3 + 2nx^3y^3,\\
D_yS_xM(\mathcal{C}_n; x, y) &= nx^2y^2 + 3nx^2y^3 + 2nx^3y^3,\\
JM(\mathcal{C}_n; x, y) &= nx^4 + 2nx^5 + 2nx^6,\\
S_xJM(\mathcal{C}_n; x, y) &= \frac{n}{4}x^4 + \frac{2n}{5}x^5 + \frac{n}{3}x^6,\\
JD_xD_yM(\mathcal{C}_n; x, y) &= 4nx^4 + 12nx^5 + 18nx^6,\\
S_xJD_xD_yM(\mathcal{C}_n; x, y) &= nx^4 + \frac{12n}{5}x^5 + 3nx^6.
\end{aligned}$$

Then, based on Table 2, the following results are obtained:

(i) $FZ(\mathcal{C}_n) = (D_x + D_y)M(\mathcal{C}_n; x, y)|_{x=y=1} = 26n$,
(ii) $SZ(\mathcal{C}_n) = (D_xD_y)M(\mathcal{C}_n; x, y)|_{x=y=1} = 34n$,
(iii) $SDD(\mathcal{C}_n) = (D_xS_y + D_yS_x)M(\mathcal{C}_n; x, y)|_{x=y=1} = \frac{31}{3}n$,
(iv) $MZ(\mathcal{C}_n) = (S_xS_y)M(\mathcal{C}_n; x, y)|_{x=y=1} = \frac{29}{36}n$,
(v) $H(\mathcal{C}_n) = 2S_xJ(M(\mathcal{C}_n; x, y))|_{x=y=1} = \frac{59}{30}n$,
(vi) $I(\mathcal{C}_n) = S_xJD_xD_y(M(\mathcal{C}_n; x, y))|_{x=1} = \frac{32}{5}n$,
(vii) $\sigma(\mathcal{C}_n) = (D_x^2 + D_y^2 - 2D_xD_y)M(\mathcal{C}_n; x, y)|_{x=y=1} = 2n$.

□

These results highlight that the regular and repetitive structure of $[n]$circulenes imposes a linear and predictable effect on the TIs, providing a robust framework for future analyses and the development of predictive models in both theoretical and applied studies.

4. Numerical and Graphical Representation

In this section, the numerical values of these TIs for $[n]$circulenes with the values of the variable n ranging from 3 to 10 are shown in Table 3, and their comparative plot is shown in Figure 3. These results provide a clear overview of how each index evolves with the increasing size of the central polygon in the $[n]$circulene structures.

Table 3. Topological indices of $[n]$circulenes for $n = 3$ to 10.

n	FZ	SZ	SDD	MZ	H	I	σ
3	78	102	31	2.4	5.9	19.2	6
4	104	136	41.3	3.2	7.8	25.6	8
5	130	170	51.6	4.0	9.8	32	10
6	156	204	62	4.8	11.8	38.4	12
7	182	238	72.3	5.6	13.7	44.8	14
8	208	272	82.6	6.4	15.7	51.2	16
9	234	306	93	7.2	17.7	57.6	18
10	260	340	103.3	8.0	19.6	64	20

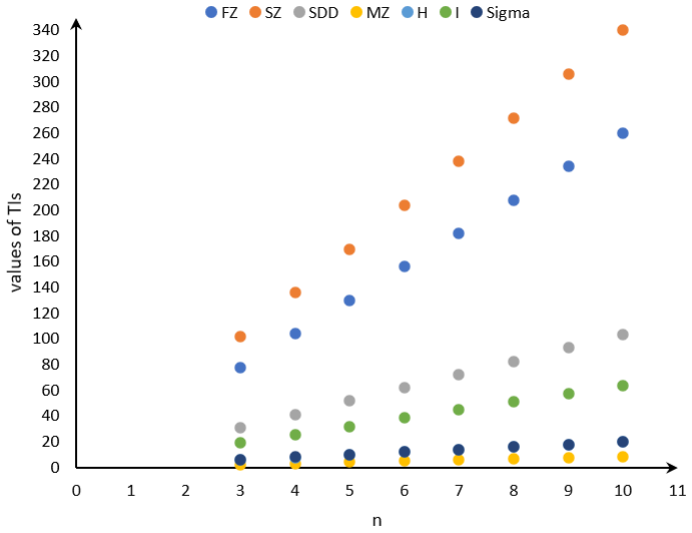

Figure 3. Comparative plots of topological indices of $[n]$circulenes for $n = 3$ to 10.

Hence, all degree-based TIs of $[n]$circulenes are linear in n, confirming the uniform structure of the graph.

According to the calculations, the values of indices for $[n]$circulenes with even and odd sizes of the central polygon are obtained from a similar formula. All studied indices exhibit an increasing trend as n increases. Notably, the σ index is exactly twice the size of the central polygon in the $[n]$circulenes. Moreover, the σ and H indices are very close, with their graphs almost overlapping, indicating a strong correlation between them. The SZ index has the highest value and the MZ index has the lowest value among the studied indices for $[n]$circulenes.

5. Asymptotic Analysis of Topological Indices of the Graph $\mathcal{C}_n$ as $n \to \infty$

The examination of the general form of the defined TIs on the graph $\mathcal{C}_n$ reveals that all of them exhibit linear growth with respect to the parameter n. More precisely, each index can be expressed in the form:

$$\text{Index}(\mathcal{C}_n) = c \cdot n,$$

Where c is a positive constant real number. This linear behavior indicates that the structure of the graph $\mathcal{C}_n$ evolves in a uniform and proportional manner with increasing graph size, reflecting consistent changes in the considered topological features. Consequently, the asymptotic behavior of these indices for large values of n is fully characterized by the coefficient c, which can be employed to compare the growth rates and sensitivities of different indices relative to the graph size, as illustrated in Figure 4.

This asymptotic analysis serves as an effective tool for understanding the behavior of TIs in large graphs and holds significant importance in molecular modeling and structure–property studies, particularly within the frameworks of QSPR and QSAR.

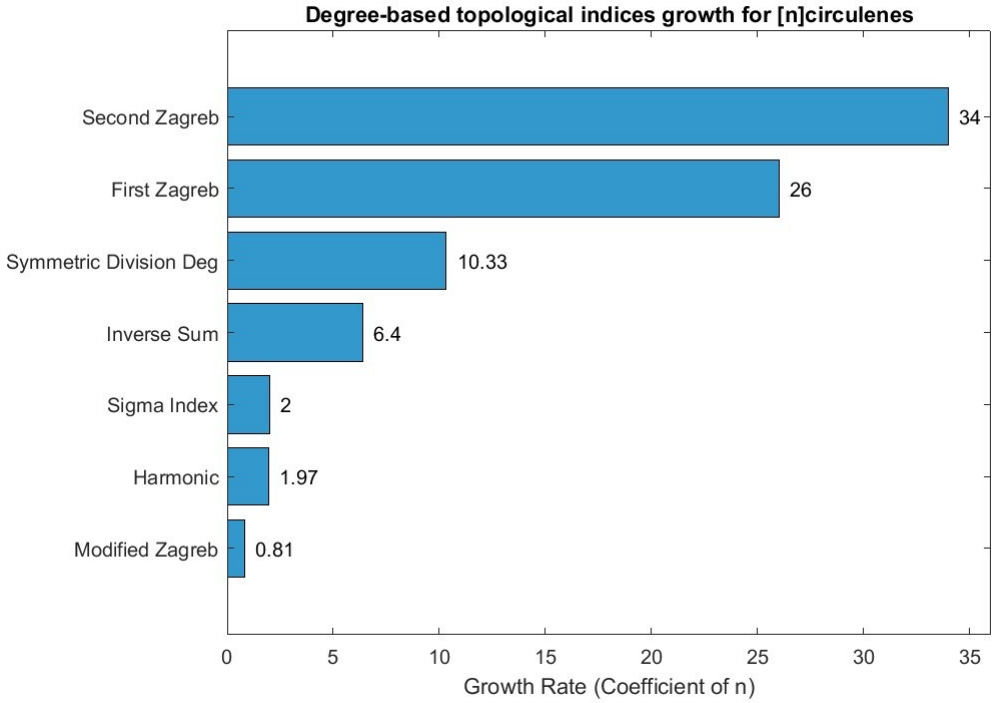

Figure 4. Growth rate of degree-based topological indices for $[n]$circulenes graphs.

The FZ and SZ indices stand out among degree-based TIs due to their notably high growth rates. The SZ index, with a growth rate of $34n$, exhibits the highest sensitivity to structural expansion. Chemically, it reflects a high local bond density and indicates the presence of strongly reactive centers within the molecular structure, making it valuable for predicting potential sites of chemical interaction.

On the other hand, the FZ index, with a growth rate of $26n$, is a general indicator of the topological stability of the structure. A significant increase in this index often suggests the localized accumulation of bonding density in specific regions of the molecule.

The SDD and I indices demonstrate moderate growth rates and play significant roles in analyzing molecular structures. The SDD index, with an approximate growth rate of

$10.33n$, is highly sensitive to bond irregularities. An increase in this index reflects the emergence of greater local asymmetries as the molecular size grows, making it particularly useful for analyzing strain centers and molecular stress. In contrast, the index I with a growth rate of 6.4 indicates a relatively slow increase in bonds between vertices with similar degrees. This reflects a heterogeneous structure with regions of side chains or sparse bonds, which plays an important role in reducing the molecule's reactivity and stability. Therefore, the molecule under study does not have a uniform distribution of vertex degrees, and areas with varying degrees are prominent.

The H, MZ, and σ indices are low-growth TIs that play important roles in analyzing the balanced and local features of molecular structures. The σ index, with a growth rate of about $2n$, measures local variations in the degrees of adjacent vertices. It is mainly useful for analyzing structural heterogeneity in small to medium-sized molecules and does not provide much overall information at larger scales. The H index, with an approximate growth rate of $1.97n$, represents the balance of vertex degrees and relative symmetry of the structure, making it suitable for describing overall stability and uniform bond distribution. The MZ index, with the lowest growth rate of about $0.81n$, is primarily used for examining local features in rings or specific parts of the structure and has limited applicability in large structures.

The growth rates of degree-based TIs for the graph $\mathcal{C}_n$ indicate that the FZ and SZ indices best reflect the structural size and are very suitable for analyzing properties dependent on bond density and site reactivity. In contrast, indices such as MZ and H, due to their lower growth rates, are more effective in analyzing the symmetry and overall stability of the structure. This information can play a crucial role in designing QSPR/QSAR models for predicting the chemical behavior of $[n]$circulenes.

6. Discussion and Conclusions

The increasing trend observed in all TIs for $[n]$circulenes (with $n = 3$ to 10) indicates a gradual enhancement in the structural complexity and topological density of these molecules. As the value of n grows, the circulene structure expands radially, increasing the number of atoms and bonds, yet maintaining a regular pattern in vertex degrees.

The σ index, which is precisely twice the size of the central polygon, corresponds to the number of degree-3 vertices. These vertices mark critical positions where the peripheral rings attach to the central core points that often play significant roles in the chemical stability and reactivity of the molecule. The closeness between the σ and H indices, both in value and in plot shape, reveals a high degree of structural symmetry and uniformity in vertex degree distribution. This is typical of highly aromatic molecules and implies stable delocalization of electrons.

The SZ index, having the largest values, emphasizes the connectivity of high-degree vertex pairs and reflects topological density. This may relate to regions of increased electron density and potential chemical activity. In contrast, the MZ index has the lowest values among the indices. This is consistent with a regular, low-degree structure with minimal variation, commonly associated with stable and chemically robust molecules.

The behavior of the SDD and I indices also supports the structural regularity and symmetry across the graph, reinforcing the idea of balanced molecular architecture.

Overall, the topological profile of $[n]$circulenes suggests a molecule that is symmetric, stable, and structurally consistent. Traits that correlate with aromaticity, predictability in reactivity, and potential utility in QSPR-based chemical modeling.

The differing growth rates of the TIs reflect their distinct sensitivities to local versus global structural features of $[n]$circulenes. Indices with higher growth rates effectively capture the influence of expanding bonding networks and potential reactive centers, whereas those with lower growth rates emphasize molecular symmetry and overall stability. Integrating indices with complementary sensitivities can enhance the predictive accuracy of QSPR/QSAR models by encompassing both local irregularities and global molecular topology.

However, this study faces certain limitations, notably the scarcity of comprehensive experimental and chemical data on $[n]$circulenes. This restricts the direct validation and correlation of topological findings with empirical observations. Future research could focus on extending the asymptotic analysis to three-dimensional molecular graphs and integrating electronic structure data or experimental findings to enhance the chemical relevance and predictive accuracy of TIs.

Despite these limitations, the presented TIs provide valuable quantitative tools that establish a robust bridge between graph theory and molecular chemistry, offering deeper insights into molecular structural characteristics and reactivity.

7. Conclusions

In this paper, general closed-form formulas for several degree-based TIs, including the FZ, SZ, SDD, I, H, MZ, and σ indices, were derived for the family of $[n]$circulene graphs based on the size of their central polygon. These formulas enable direct and efficient computation of the indices without the need for complex edge partitioning or exhaustive enumeration.

Numerical and graphical analyses show a consistent linear increase in all indices with the growth of the parameter n, indicating a proportional rise in the structural complexity and topological richness of $[n]$circulenes. The SZ index had the highest value, while the FZ index had the lowest. Furthermore, the strong correlation observed between the σ and H indices reflects the high symmetry and uniform vertex degree distribution characteristic of these molecules.

Moreover, the asymptotic analysis reveals that although all indices grow linearly, their differing growth rates reflect varying sensitivities to molecular structural features. The SZ and FZ indices, which have the highest growth rates, effectively capture the increase in bonding density and reactive centers, making them very useful for predicting chemical activity and molecular stability. Indices with moderate growth rates, such as SDD and I, reveal local asymmetries and heterogeneities that are important for understanding molecular strain and reactivity, while indices with lower growth rates, such as H, MZ, and σ, emphasize global symmetry and structural balance.

This comprehensive mathematical framework not only provides valuable insights into the topological properties of $[n]$circulenes but also enhances their applicability in quantitative structure–property relationship (QSPR) modeling. Despite current limitations due to the lack of extensive experimental data for validation, the closed-form analytical formulas presented in this study facilitate faster and simpler computation of TIs and advance both the theoretical understanding and practical use of graph-based molecular descriptors.

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Zohreh Rajabinejad obtained her BSc in Applied Mathematics and her MSc in Numerical Analysis. She is currently pursuing a Ph.D. in Applied Mathematics at Semnan University, Iran. Her primary research interests lie in graph theory and its applications. She has authored and co-authored several research papers published in ISI and ISC-indexed journals, and has presented her work at various national and international conferences.

Dr. Saeed Mohammadian Semnani is an Associate Professor in the Department of Mathematics at the Faculty of Mathematics, Statistics, and Computer Science, Semnan University, Iran. He received his BSc in Applied Mathematics from Ferdowsi University of Mashhad, his MSc in Applied Mathematics with a specialization in Operations Research from Tarbiat Modares University, Tehran, and his Ph.D. in Graph Theory from Iran University of Science and Technology. His research interests include ordinary differential equations, numerical computations, and graph theory. He has co-authored several textbooks in Persian, including Numerical Computations (2001, with Bagher Karamati) and Ordinary Differential Equations and Their Applications (2020, with Milad Mahdavi). He has published numerous papers in national and international journals indexed in ISC and ISI, and has actively participated in academic conferences.