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Improved Methods for Determining the Topological Indices of [n] Circulenes from the Central Polygonal Area

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Abstract

Many researchers in computational and theoretical chemistry are fascinated by the structures of circlenes, which are unusual cyclic compounds generated by alternating polygonal bonds. Their geometric and topological features are particularly noteworthy. Numerous domains, such as materials science, nanochemistry, and medicines, make use of these structures. For [n] circulenes, new formulae for distance-based topological indices are given in this study. By doing away with the need for edge partitioning, these formulae hope to streamline and quicken the computation process. If one knows the size of the center polygon in the circulon structure, they may simply compute the index using the general formulae supplied for the Szeged, Mostar, and PI indices. There is a graphical comparison of several topological indices and numerical findings are also provided. Additionally, we investigate the possible relationship between these indices and certain physicochemical features of [n] circulenes. Along with the indexes' maximum and minimum values, we also provide the index that, relative to the others, has the strongest link to the physicochemical attributes. These results are helpful for future research since they do not need polynomials to be calculated.

Keywords: Structural matrix polynomial, molecular graph, [n] circulenes, distance-based topological index, Szeged index, Mostar index, PI index Value of the correlation

1. Introduction

Polycyclic aromatic hydrocarbons known as circlenes have an aromatic ring in the middle with n fused benzenoid rings around it. See Figure 1 for an illustration of how this type of molecules is designated [n] circulenes, after the number of benzene rings that round the core, which is proportional to the size of the center polygon. [n] Between the values of 3 and 5, circulenes have a bowl form with positive curvature, but between the values of 7 and 16, they take on a saddle shape with negative curvature [1, 2]. When n is 17 or more, its topography takes on a helical shape [3]. Because of their aromaticity, chiroptical characteristics, electrical and optical properties, electrochemical behavior, and potential uses in nanophotonics, hydrogen storage, and other fields, circulenes have piqued the curiosity of several chemists [1, 2, 4, 5].

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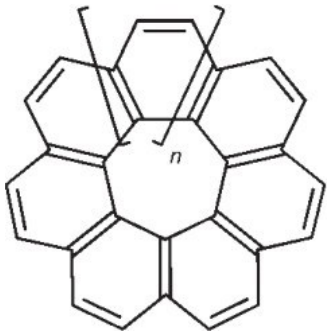

Figure 1: Structure of [*n*] circulene.

One mathematical subfield that bridges the gap between graph theory and chemical science is known as chemical graph theory. Molecular graphs, with atoms at the nodes and chemical bonds at the edges, are the standard representation of molecules in this area of study [6, 7]. To determine the molecular structure and topology, scientists apply a variety of graph theory methods. Chemical compound properties, such boiling temperature, may be predicted, for instance, by observing the degree and distance between its vertices. As a result, the mathematically-analyzed useful properties of the linked chemical compound are strongly influenced by the topology of the molecular structure. With this method, molecular structure may be used to analyze chemical characteristics more precisely, and it has several uses in chemical compound prediction and engineering [8]. Numerical quantities known as topological indices (TIs) may be used to forecast the chemical, biological, and physical characteristics of molecular structures [6]. TIs are used to quantify the topological similarity of chemical compounds [9]. They include numerical information on molecule size, shape, and branching. Variables like eigenvalues, vertex degree, and distance between pairs of vertices determine TIs. The Wiener index, for instance, is strongly associated with a number of molecular structures' physical and chemical characteristics, and it is among the most used distance-based indices [10]. Information about the molecular graph may be more easily provided by calculating the topological polynomials instead of molecular descriptors.

M, NM, SMP, and Hosoya polynomials are among the polynomials. The M-polynomial was defined by Deutsch and Klavzar in 2015. To forecast the chemical characteristics of nanostructures and polycyclic aromatic hydrocarbons, among other chemical structures, scientists have turned to the degree-based polynomial known as M-polynomial [11, 12]. A vertex's NM-polynomial is defined as the sum of its neighbours' degrees [6, 13]. A polynomial belonging to the domain of distance-based TIs is the Hosoya polynomial. It is possible to generate almost all distance-based TIs from this polynomial. Numerous chemical processes make use of the Hosoya polynomial [14].

A novel graph polynomial, the SMP-polynomial, was presented in 2023 by Knor and Tratnik. It makes it easier to calculate a number of TIs, such as the Szeged (Sz), Mostar (Mo), and PI indices. A useful tool in the study of chemical behaviors and characteristics, TIs correlate with biological activities and chemical properties, increasing the molecular descriptor's prediction potential [15, 16].

Graphs' Cartesian products are where the SMP-polynomial shines. Its capacity to simplify the process of deriving characteristics from coupled graph topologies is what sets it apart from other polynomials [17]. The structure of hyaluronic acid, which is significant in medicinal applications, is one example of a biological system that this polynomial is utilized in [15, 17]. It is also used in computer science, network theory, chemistry, and materials research. Here is the SMP-polynomial G: [17]

$$SMP(G;x,y) = \sum_{e=uv\in E(G),\, n_u(e|G)\geq n_v(e|G)} x^{n_u(e|G)}y^{n_v(e|G)}.$$

where $N_u(e|G) = \{x \in V(G)|d_G(x,u) < d_G(x,v)\}$ is a set of vertices of G lying closer to u and $n_u(e|G) = |N_u(e|G)|$ is the number of this set of vertices.

The advantage of the mentioned polynomial is that to calculate Sz, Mo, and PI indices, instead of calculating the three polynomials Sz, Mo, and PI, only the SMP-polynomial is calculated [18].

Khadikar introduced the Padmakar-Ivan TI. Padmakar-Ivan index is denoted as PI. Ashrafi defined the PI vertex index. Ivan Gutman introduced the Sz index, which is a distance-based index. Sz index is the oldest TI based on

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distance and is as follows [19, 20]:

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e|G) n_v(e|G).$$

Mo index is as follows [21]:

$$Mo(G) = \sum_{e=uv \in E(G)} |n_u(e|G) - n_v(e|G)|.$$

Khadikar introduced the vertex PI index as follows:

$$PI_v(G) = \sum_{e=uv \in E(G)} (n_u(e|G) + n_v(e|G)).$$

The focus here has shifted from earlier efforts in chemical graph theory and TIs to investigating other topological descriptors for molecular structures, with a special emphasis on cyclic graphs and other chemical compounds. In order to forecast physical and chemical characteristics, these types of research often use polynomials like the M-polynomial, Hosoya polynomial, Schultz polynomial, and modified Schultz polynomial to determine TIs. Furthermore, a number of issues in graph theory have been tackled in some research by using algebraic methods [22, 8].

Using tools including degree-counting techniques, vertex and edge splitting methods, and combinatorial approaches, Nadeem et al. studied the interaction between non-isomorphic pseudo-divisor graphs and a certain class of rings G. A number of TIs depending on degree, distance, and degree-distance were computed by using structural features of quasi-divisor graphs [23]. In addition, using the degree 2-dimensional silicon-carbon compounds Si2C3 − III and SiC3 − III, they calculated precise values for topological descriptors [24]. Though efficient, these approaches often need sophisticated computations, which in turn necessitates edge splitting to extract graph-related information and may be rather time-consuming. On the other hand, the recently suggested SMP-polynomial is introduced in this paper and is especially useful for Cartesian product graphs. By combining the computation of many polynomials into a single operation, this approach improves the efficiency and precision of the computations. Also, in the [n] circulenes structure, the size of the center polygon is all that is needed to compute distance-based indices like Sz, Mo, and PI using SMP-polynomials. This eliminates the need for edge partitioning and drastically streamlines the computing procedure. This study differs mainly from its predecessors in that it employs an efficient method based on SMP-polynomials. The computational time required to forecast the chemical and physical characteristics of molecular compounds has been significantly reduced because to this invention. A major step forward in making topological analysis more accessible and useful in theoretical and computational chemistry has been made in this work.

An overview of [n] circulene structure and its relevance to computational and theoretical chemistry is provided at the beginning of this work. An exhaustive account of the research procedure, including all instruments and procedures, is given in the second part. In the third part, we look at the ways that new formulae for distance-based TIs of [n] circulenes were derived. In the fourth part, we compare our findings to those of other methodologies and provide numerical and graphical representations of the results. Section 5 presents statistical studies that explore the relationships between the indices and the physicochemical characteristics of certain circulenes, illuminating their real-world uses. At the end of the study, the key points are reviewed along with recommendations for where the research should go from here.

2. Methodology

This article delves into the construction of [n] circulenes and their distance-based TIs. The polygonal bonding patterns of these cyclic compounds are the primary focus of the first geometric analysis. Next, the circulene compound is partitioned along edges according to the number of vertices that are closer to each end of the edges. This process yields the SMP-polynomials. By using these polynomials, new distance-based TI calculation algorithms are obtained, which are size-dependent only. By using these formulae, edge partitioning is no longer necessary, and the calculating procedure is made much simpler. We compare several TIs and provide the findings quantitatively and visually. In the end, statistical tests are run to find out which TI indices correlate best with the physicochemical features of [n] circulenes, and how the TIs relate to these qualities. The TIs of [n] circulenes are studied and calculated using these approaches in a thorough and efficient manner, illuminating its real-world computational and theoretical chemistry applications.

3. Main Results

Let G be the base graph of $[n]$ circulenes with $4n$ vertices and $5n$ edges. The number of vertices, edges, and size of the central polygon are denoted by p, q, and n, respectively. Some distance-based TIs computed via the SMP-polynomial are presented in Table 1. The edge partitioning of the graph is shown in Tables 2 and 3. These tables include the total number of vertices, the total number of edges, the size of the central polygons, the different types of edges, and the count of each edge type.

Table 1: Derivation of some TIs from SMP-polynomial.

Topological index	Derivative from $SMP(G; x, y)$
Sz index	$D_x(D_y(SMP(G; x, y))\|_{x=y=1}$
Mo index	$D_x(SMP(G; x, \frac{1}{x}))\|_{x=1}$
PI index	$D_x(SMP(G; x, x))\|_{x=1}$

Table 2: Edge partition of $[n]$ circulenes where n is even, where $n \geq 4$.

Type of edges	$(4n-5, 5)$	$(2n, 2n)$	q	p
Number of edges	$3n$	$2n$	$5n$	$4n$

Table 3: Edge partition of $[n]$ circulenes when n is odd, where $n \geq 5$.

Type of edges	$(4n-5, 5)$	$(\frac{3n+1}{2}, \frac{3n+1}{2})$	q	p
Number of edges	$3n$	$2n$	$5n$	$4n$

Theorem 3.1. *Let G be the base graph of $[n]$ circulenes when n is even, where $n \geq 4$. Then, the SMP-polynomial of G is as follows:*

$$SMP(G; x, y) = 3nx^{4n-5}y^5 + 2nx^{2n}y^{2n}.$$

Proof. Using Table 2, the SMP-polynomial of G is calculated as follows:

$$SMP(G; x, y) = \sum_{n_u(e|G) \geq n_v(e|G)} x^{n_u(e|G)}y^{n_v(e|G)} = |E_{(4n-5,5)}|x^{4n-5}y^5 + |E_{(2n,2n)}|x^{2n}y^{2n} = 3nx^{4n-5}y^5 + 2nx^{2n}y^{2n}.$$

□

Proposition 3.2. *Consider the $[n]$ circulenes structure, where n is even. Then, TIs of G are obtained as follows:*

(i) $Sz(G) = 8n^3 + 60n^2 - 75n$,
(ii) $PI(G) = 20n^2$,
(iii) $Mo(G) = 12n^2 - 30n$.

Proof. Let $SMP(G; x, y) = 3nx^{4n-5}y^5 + 2nx^{2n}y^{2n}$. Using Table 1, the following results are obtained by applying the operators on the SMP-polynomial:

$$D_ySMP(G; x, y) = 15nx^{4n-5}y^4 + 4n^2x^{2n}y^{2n-1},$$

$$D_xD_ySMP(G; x, y) = 15n(4n-5)x^{4n-6}y^4 + 8n^3x^{2n-1}y^{2n-1},$$

$$D_xSMP(G; x, \tfrac{1}{x}) = (12n^2 - 30n)x^{4n-11},$$

$$D_xSMP(G; x, x) = 20n^2x^{4n-1}.$$

Then, according to Table 1, we conclude that:

(i) $Sz(G) = D_xD_ySMP(G;x,y)|_{x=y=1} = 8n^3 + 60n^2 - 75n$,
(ii) $PI(G) = D_xSMP(G;x,x)|_{x=1} = 20n^2$,
(iii) $Mo(G) = D_xSMP(G;x,\frac{1}{x})|_{x=1} = 12n^2 - 30n$.

□

Theorem 3.3. *Let G be the base graph of* [n] *circulenes when n is odd, where* $n \geq 5$. *Then, the SMP-polynomial of G is as follows:*

$$SMP(G;x,y) = 3nx^{4n-5}y^5 + 2nx^{\frac{3n+1}{2}}y^{\frac{3n+1}{2}}.$$

Proof. Using Table 3, the SMP-polynomial of G is calculated as follows:

$$SMP(G;x,y) = \sum_{n_u(e|G)\geq n_v(e|G)} x^{n_u(e|G)}y^{n_v(e|G)} = |E_{(4n-5,5)}|x^{4n-5}y^5 + |E_{(\frac{3n+1}{2},\frac{3n+1}{2})}|x^{\frac{3n+1}{2}}y^{\frac{3n+1}{2}} = 3nx^{4n-5}y^5 + 2nx^{\frac{3n+1}{2}}y^{\frac{3n+1}{2}}.$$

□

Proposition 3.4. *Consider the* [n] *circulenes structure, where n is odd. Then, TIs of G are obtained as follows:*

(ii) $Sz(G) = \frac{1}{2}(9n^3 + 126n^2 - 149n)$,
(ii) $PI(G) = 18n^2 + 2n$,
(iii) $Mo(G) = 12n^2 - 30n$.

Proof. Let $SMP(G;x,y) = 3nx^{4n-5}y^5 + 2nx^{\frac{3n+1}{2}}y^{\frac{3n+1}{2}}$. Using Table 1, the following results are obtained by applying the operators on the SMP-polynomial:

$$D_y SMP(G;x,y) = 15nx^{4n-5}y^4 + n(3n+1)x^{\frac{3n+1}{2}}y^{\frac{3n+1}{2}-1},$$

$$D_x D_y SMP(G;x,y) = (60n^2 - 75n)x^{4n-6}y^4 + \frac{n(3n+1)^2}{2}x^{\frac{3n+1}{2}-1}y^{\frac{3n+1}{2}-1},$$

$$D_xSMP(G;x,\tfrac{1}{x}) = (12n^2 - 30n)x^{4n-11},$$

$$D_xSMP(G;x,x) = 12n^2x^{4n-1} + (6n^2 + 2n)x^{3n}.$$

Then, according to Table 1, we conclude that:

(i) $Sz(G) = D_xD_ySMP(G;x,y)|_{x=y=1} = \frac{1}{2}(9n^3 + 126n^2 - 149n)$,
(ii) $PI(G) = D_xSMP(G;x,x)|_{x=1} = 18n^2 + 2n$,
(iii) $Mo(G) = D_xSMP(G;x,\frac{1}{x})|_{x=1} = 12n^2 - 30n$.

□

4. Numerical and Graphical Representation

With n values between 4 and 12, Table 4 displays the numerical values of these TIs for [n] circulenes. Using the same approach, the computations show that the Mo index values for [n] circulenes with even and odd central polygon sizes can be derived. Figure 2 shows the visual depiction of this index. For [n] circulenes with even and odd diameters of the central polygon, one uses a different formula to get the value of the Sz and PI indices. These indexes are shown graphically in Figures 3 and 4. Every one of these TIs is absolutely rising, with the exception of the Sz. While the Sz index does rise between 4 and 10, it does not become monotone when n is more than 10. When it comes to [n] circulenes, the Sz index is at the top of the list and the Mo index is at the bottom.

Table 4: Numerical comparison of $PI(G)$, $Mo(G)$, and $Sz(G)$.

n	4	5	6	7	8	9	10	11	12
$Sz(G)$	1172	1765	3438	4109	7336	7713	13250	12793	21564
$PI(G)$	320	460	720	896	1280	1476	2000	2200	2880
$Mo(G)$	72	150	252	378	528	702	900	1122	1368

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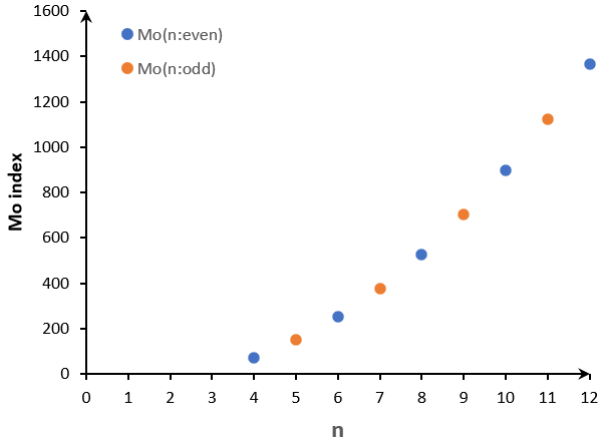

Figure 2: Comparison of Mo index when the size of the central polygon of [*n*] circulenes is even or odd.

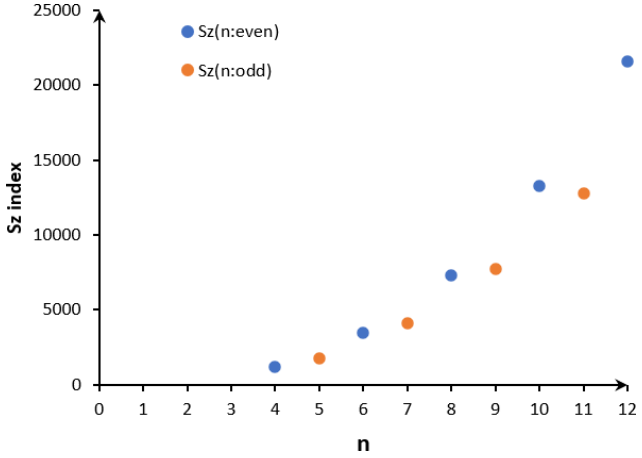

Figure 3: Comparison of Sz index when the size of the central polygon of [*n*] circulenes is even or odd.

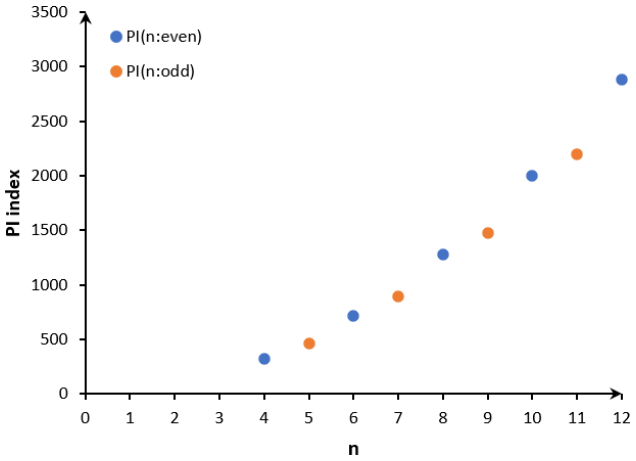

Figure 4: Comparison of PI index when the size of the central polygon of [*n*] circulenes is even or odd.

5. Statistical Analysis and Applications

Here we look at some real-world applications and correlations between the physicochemical features of [n] circulenes and indices for different values of n. Referring to Figure 5, this section discusses the topic's applications for circulene [5], circulene [6], and circulene [7]. Because there is experimental evidence for their different characteristics, these circulenes were chosen as test molecules. Due to its unusual geometric and topological features, circulenes—unique cyclic structures made of alternating benzene bonds—have garnered a lot of interest from the chemical and computational communities. Polycyclic aromatic hydrocarbons having five benzene rings fused to one cyclopentane ring are known as circulene (C20H10), corannulene, or buckybowl. The scientific community is interested in corannulene because of its possible uses in energy storage and solar cells, among others [25, 26]. The chemical formula for coronene is C24H12. It is a polycyclic aromatic hydrocarbon (PAH) having a planar, hexagonal structure made up of seven fused benzene rings. Coronanene is a common model system for studying the characteristics of different aromatic compounds because of its well defined and relatively simple structure. The electrical, optical, and chemical properties of coronene, which is well-known for its fluorescence, have been the focus of much investigation. Theoretical and experimental investigations use it as a reference molecule as well [27].

In terms of negative Gaussian curvature, the [7] circulene (C28H14) is the smallest saddle-shaped [n] circulene. The induced planarization of extremely curved π-systems has garnered significant attention in recent studies because to the substantial impact planarization has on their electrical characteristics [28].

Molecular weight (MW), XlogP3, and complexity are some of the physicochemical parameters that are examined in this research. When it comes to chemical reactions and processes, molecular weight is a major factor that determines how materials behave and how reactive they are [29]. Understanding molecular behavior and attributes requires research into chemical structures, namely XlogP3 and complexity. XlogP3 measures lipophilicity, which is important for drug design and materials research, and shows how effectively a chemical dissolves in non-polar settings. New studies show that the amount of rings and links in a molecular structure, among other parameters, greatly affects its lipophilicity and reactivity. To better anticipate how a molecule will behave in biological systems, for example, and to build more efficient nanomaterials and medicines, it is helpful to consider the relationship between structural complexity and physicochemical characteristics. Researchers may improve the effectiveness and safety of substances in areas like medicine development and environmental chemistry by understanding these interactions [30, 31, 32].

Complexity, XlogP3, and MW were chosen for the comparison testing because of the significance of these traits. Table 5 displays the physicochemical characteristics of these circulenes which were retrieved from PubChem and ChemSpider. The compounds' measured Mo, Sz, and PI indices are also shown in Table 4. Table 6 displays the correlation coefficients obtained by comparing the indices with the physicochemical parameters. With a value of r = 0.9939369, the PI index has the most robust positive connection with MW. Furthermore, when it comes to emulating MW, XlogP3, and Complexity, the PI index is the clear winner. While XlogP3 and Complexity provide dependable results from the Sz index, MW does not. Sz and MW seem to have a weak linear connection, as shown by the modest correlation coefficient. The regression model may have failed to adequately reflect the link between other parameters and changes in Sz, as this suggests. On the other hand, none of the assessed traits can be reliably predicted by the Mo index.

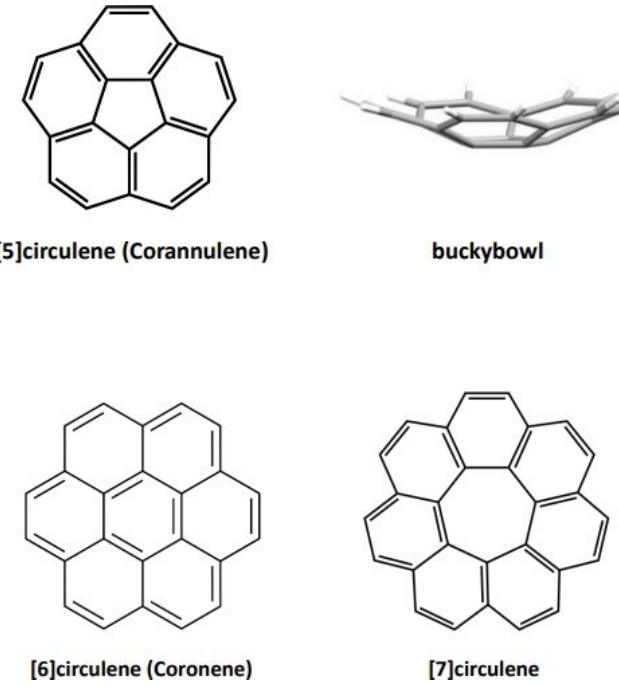

Figure 5: Chemical structures of [5], [6], and [7] circulenes

Table 5: physicochemical properties of [*n*] circulenes.

[*n*] Circulene	Molecular weight	XlogP3	Complexity
[5] Circulene	250.3	6	303
[6] Circulene	300.4	7.2	376
[7] Circulene	350.4	8.5	451

Table 6: The correlation between PI, Sz, Mo, and physicochemical properties of [*n*] circulenes.

Indices	Molecular weight	XLog P_3	Complexity
PI	0.9939369	0.9909363	0.9929790
Sz	0.0009710	0.9649438	0.9689712

Using the generic formulae that were acquired to calculate the Sz, Mo, and PI indices is advantageous since it simplifies and speeds up the computation process by doing away with edge segmentation and polynomial calculations. In addition, the numerical and graphical representations of the data are quite helpful in understanding the indices' behavior and how it relates to the physicochemical characteristics. The PI index is most positively correlated with parameters like MW, XlogP3, and complexity, according to correlation study. These qualities may be used for molecular behavior prediction and material design. On the other hand, there are certain drawbacks to this work. Specifically, neither the Sz nor the Mo indices have been able to adequately represent molecular characteristics; furthermore, the Mo index has shown to be unreliable across all assessed features. In addition, although the indicators are compared numerically and graphically, there is no in-depth examination of how they change under more particular circumstances or on scales outside the samples that were investigated.

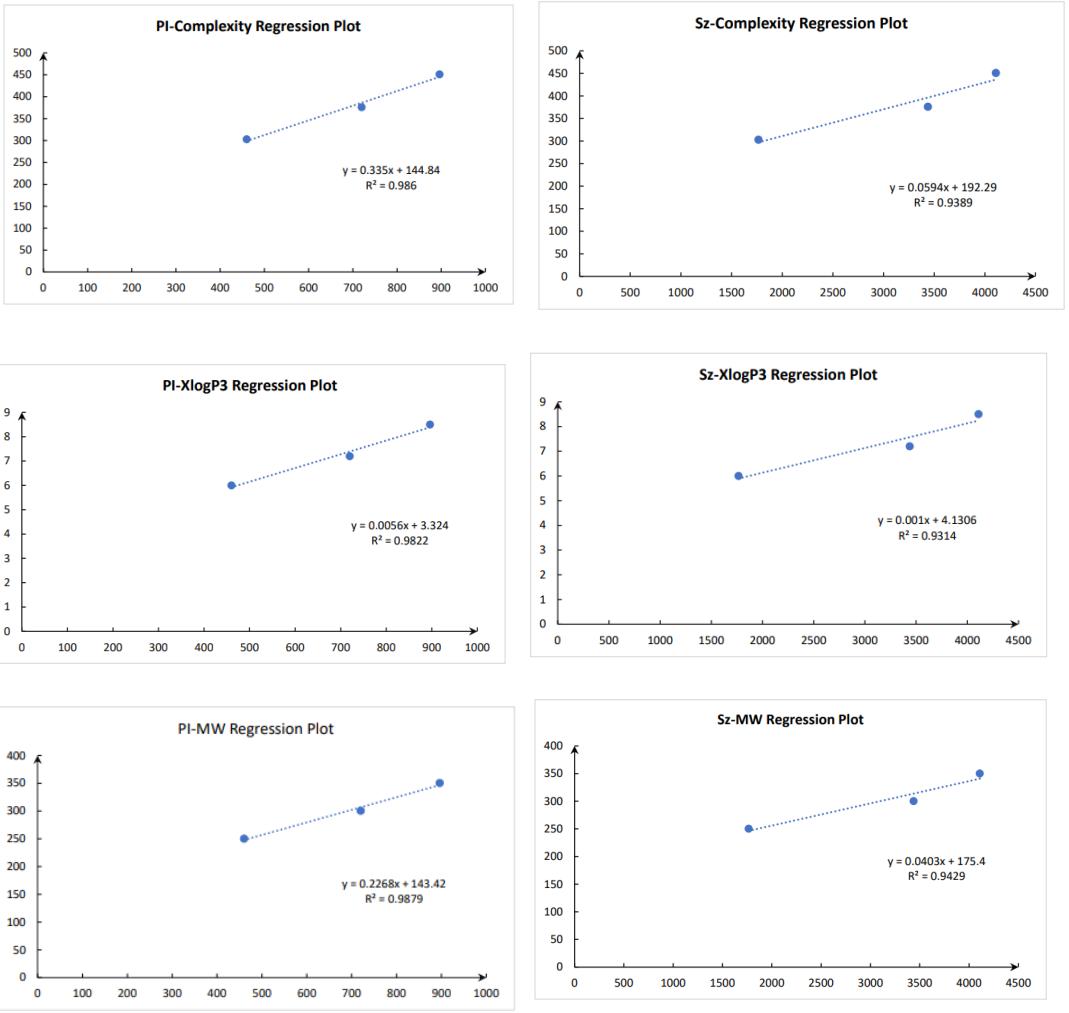

Figure 6: Regression Plots.

6. Conclusion

This article presents general formulae for the Sz, Mo, and PI indices that are derived from the size of the central polygon of [n] circulenes. You can calculate indices using these formulae without having to segment the edges. The findings are shown numerically and visually. All of these indexes, with the exception of the Sz, are going up. Monotone does not describe the Sz index. The Mo index is the most highly ranked of the studied indices for [n] circulenes, while the Sz index is the least ranked. The chemical and physical characteristics of structures may be better understood with the help of these indexes. Since no polynomials are used, these findings are appropriate for use in further investigations. Indexes and physicochemical parameters were analyzed for association, and the PI index was shown to have the highest positive link with physical and chemical characteristics in comparison to other benchmarks. Figure 6 shows that a significant amount of the index fluctuation has been well explained by the regression models. These models have great predictive capacity and can explain the changes in the data, as seen by their high R values. These outcomes indicate that the models have made good use of the given data to forecast the indexes.

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