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Research Paper

New formulas for distance-based indices of Helicenes via benzene rings and their correlation with physicochemical properties

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Abstract. Helically-shaped chiral molecules are produced when benzene rings are angularly annulated to form Helicenes. Helicenes are ortho-condensed polycyclic aromatic compounds with the chemical formula $C_{4n+2}H_{2n+4}$ that have received attention due to their distinct structural, spectral, and optical properties, alluring physicochemical properties, and their application in various research fields. In this article, novel formulas of Szeged, Padmakar-Ivan, and Mostar indices are obtained through SMP-polynomials for Helicenes. These formulas do not need to count edges and can be calculated based on the number of benzene rings of Helicenes. Then, the results are displayed numerically and graphically and the topological indices are compared. Finally, the study explores the correlation between these indices and several physicochemical characteristics of different helicenes.

Keywords. Helicenes, SMP-polynomial, Szedeg index, Mostar index, Padmakar-Ivan index, Correlation coefficient

Mathematics Subject Classification (2010): 05C31, 05C92, 05C09, 05C30, 05C90.

1 Introduction

Spiral staircases, vines, microtubules, and double-stranded DNA are just a few examples of the many helical structures found in nature. These structures, which can range in size from

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the nanometer to meter order, serve a variety of functions that are directly tied to their helical structures. The study of tiny molecules with helical architectures is therefore intriguing. Since many biomacromolecules, including proteins and nucleic acids, have helical structures, the interaction of small helical molecules can be a creative way to create new biologically active substances. A class of polycyclic aromatic compounds known as helicenes (H) have helical shapes that result from steric repulsions, usually between the terminal aromatic rings. Chemists have been interested in these chiral polycyclic hydrocarbons for many years, not only because of their stunning $3D$ helical topology that artificially mimics natural helical structures like double-stranded DNA or snail shells but also because of their many alluring physicochemical properties and subsequent applications in various research areas [1].

According to the number of rings in the structure, H with the general formula $C_{4n+2}H_{2n+4}$ is systematically named: The structure with n rings is called $[n]$ helicene. By definition, IUPAC only considers structures to be helices if n is at least 5. The structure is not flat after the first four rings and instead, the planes of the subsequent rings tilt to prevent steric collisions. Figure 1 shows a chiral helix. Rajabinejad et al. investigated some topological indices (TIs) of the linear and zigzag structure of polyacenes [2,3].

The progress of the chemical sciences is significantly influenced by the mathematical chemistry subfield known as chemical graph theory. Mathematical models of chemical structures based on polynomials can be used to calculate tools like polynomials, which can then be used to forecast the physical and chemical properties of a substance. One of the most active areas of research in chemical graph theory at the moment is the study of TIs can be used to predict a variety of chemical and biological characteristics of chemical structures. TIs are utilized to create qualitative structure-activity connections and provide a numerical description of molecular structure.

Topological polynomials are used in mathematical chemistry for calculating TIs. Calculating the topological polynomials rather than the computation of TIs facilitates the provision of information regarding the molecular graph. Various polynomials have been developed for graphs, including M and MN polynomials. In 2015, Deutsch and Klavzar defined the M-polynomial as a degree-based polynomial used to predict the chemical properties of various structures, including nanostructures and polycyclic aromatic hydrocarbons [4,5]. The NM polynomial, which depends on the sum of adjacent vertex degrees, is another key tool in chemical structure analysis [6,7]. Additionally, polynomials corresponding to the Szeged (Sz), Mostar (Mo), and Padmakar-Ivan (PI) indices have been defined. These indices can be obtained by evaluating the first derivative of the respective polynomials at $x = 1$. A new polynomial of two variables was introduced by Knor and Tratnik, which is called the SMP polynomial; the Sz, Mo, and PI indices can be easily calculated via this polynomial. The advantage of the SMP polynomial is that to compute these indices, only one polynomial can be considered instead of three polynomials [6,8–10].

Atoms and bonds are depicted, respectively, as vertices and edges in chemical graphs [11]. Numerous scientific fields, including material science, mathematics, computing, biology, etc., can benefit from applying the TIs. The non-exact quantitative structure-property and quan-

titative structure-activity links, however, are where TIs are currently being used most crucially [12]. There are various types of indices, including distance-based TIs and indices based on degree. In reality, these are the numerical values that link the structure to different physical attributes, chemical reactivity, and biological activities. It is well known that several aspects of a molecule, including its heat of formation, boiling point, strain energy, rigidity, and fracture toughness, are closely related to its graphical structure. In calculating TIs, the SMP-polynomial, Hosoya polynomial, and Wiener polynomial all play crucial roles. Since Harry Wiener first developed his now-famous index in the 1940s, distance-based topological indices have been applied to the study of molecular graphs. Several tens of these indices are currently being actively researched in the literature on mathematical chemistry [8,9,11].

Harold Wiener introduced the Wiener index, The Wiener index $W(G)$ is as:

$$W(G) = \sum_{u,v \in V(G)} d_G(u,v). \tag{1}$$

Notice that where G is a connected graph. The Wiener index for tree T can be calculated as:

$$W(T) = \sum_{e=uv \in E(T)} n_u(e|T) n_v(e|T). \tag{2}$$

where $n_u(e|T)$ signifies the number of vertices of T whose distance to u is smaller than the distance to v. Similarly, we define $n_v(e|T)$. The Sz index using (2) was introduced by Gutman in 1994 [8]. The Sz index is as follows [9,13]:

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e|G) n_v(e|G). \tag{3}$$

The PI index was proposed by Khadikar in 2000. Khadikar et al. his coauthors investigated the chemical and biological application. It is a TI for measuring graph properties. It can be applied to perfect graphs, including co-bipartite and line. The vertex PI index is a variation of the index that focuses on the vertices of the graph and their distances from each other [14].

The vertex-PI index as [15]:

$$PI_v(G) = \sum_{e=uv \in E(G)} (n_u(e|G) + n_v(e|G)). \tag{4}$$

The Mo is defined as [16]:

$$Mo(G) = \sum_{e=uv \in E(G)} |n_u(e|G) - n_v(e|G)|. \tag{5}$$

The SMP-polynomial of G is as:

$$SMP(G,x,y) = \sum_{e=uv \in E(G), n_u(e|G) \geq n_v(e|G)} x^{n_u(e|G)} y^{n_v(e|G)}. \tag{6}$$

where $N_u(e|G) = \{x \in V(G)|d_G(x,u) < d_G(x,v)\}$ and $n_u(e|G) = |N_u(e|G)|$ that is the number of vertices of G lying closer to u, see [13].

The indices can be determined either through edge partitioning or via the SMP-polynomial, as outlined in Table 1. In the next section, Sz, Mo, and PI indices of helicene are calculated through new formulas without edge partitioning. These formulae only require the number of benzene rings.

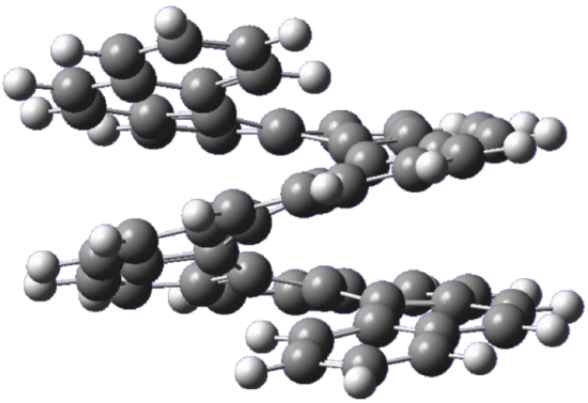

Figure 1. Molecular structure [13]helicene.

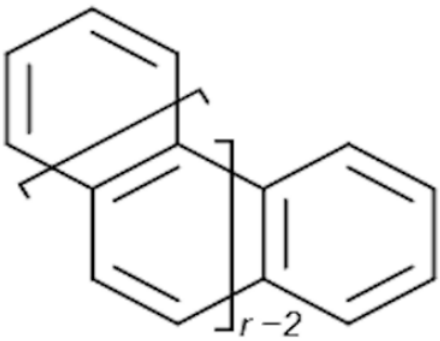

Figure 2. General structure formula of $[r]$helicene, $r \geq 5$.

2 Results and Discussion

In this paper, G is the base graph of Helicene with $4r + 2$ vertices and $5r + 1$ edges, see Figure 2. The number of vertices, edges, and benzene rings in this structure are denoted by n, m, and r, respectively. Notice that only structures for which r is at least 5 are classified as

helices by IUPAC.

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

TI	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. Edges partition of H, when r is even.

$\{n_u,n_v\}$	Number of edges
$\{4r-1,3\}$	8
$\{4r-3,5\}$	$3r-3$
$\{4r-4k-5,7+4k\}$	$2r-4$
Total edges	$5r+1$
$r\geq 5,\ 0\leq k\leq \frac{r-4}{2}$.	

Table 3. Edges partition of H, when r is odd.

$\{n_u,n_v\}$	Number of edges
$\{4r-1,3\}$	8
$\{2r+1,2r+1\}$	2
$\{4r-3,5\}$	$3r-3$
$\{4r-4k-5,7+4k\}$	$2r-6$
Total edges	5r+1
$r\geq 5,\ 0\leq k\leq \frac{r-5}{2}$.	

Theorem 2.1. *Let H when r is even, $r\geq 5$. Then, its SMP-polynomial is as follows:*

$$SMP(H;x,y)=8x^{4r-1}y^3+3(r-1)x^{4r-3}y^5+4\sum_{k=0}^{\frac{r-4}{2}}x^{4(r-k)-5}y^{7+4k}.$$

Proof. By using Figure 2 and Table 2, we calculate the SMP-polynomial of H as follows:

$$\begin{aligned}SMP(H;x,y) &= \sum_{e=uv\in E(G), n_u(e)\geq n_v(e)} x^{n_u(e|G)}y^{n_v(e|G)}\\ &= |E_{\{4r-1,3\}}|x^{4r-1}y^3 + |E_{\{4r-3,5\}}|x^{4r-3}y^5 + |E_{\{4r-5,7\}}|x^{4r-5}y^7\\ &+ \ldots + |E_{\{2r+3,2r-1\}}|x^{2r+3}y^{2r-1} = 8x^{4r-1}y^3 + 3(r-1)x^{4r-3}y^5\\ &+ 4x^{4r-5}y^7 + \ldots + 4x^{2r+3}y^{2r-1} = 8x^{4r-1}y^3 + 3(r-1)x^{4r-3}y^5\\ &+ 4\sum_{k=0}^{\frac{r-4}{2}} x^{4(r-k)-5}y^{7+4k}.\end{aligned}$$

□

Proposition 2.2. *Consider H when r is even, then the following holds:*

- $Sz(H) = \frac{1}{3}(16r^3 + 204r^2 - 157r + 99)$,
- $PI(H) = (5r+1)(4r+2)$,
- $Mo(H) = 16r^2 - 20r + 8$.

Proof. Let $SMP(H;x,y) = 8x^{4r-1}y^3 + 3(r-1)x^{4r-3}y^5 + 4\sum_{k=0}^{\frac{r-4}{2}} x^{4(r-k)-5}y^{7+4k}$. The following results are obtained by applying the operators on the SMP-polynomial.

$$\begin{aligned}D_xD_ySMP(H;x,y) &= 24(4r-1)x^{4r-1}y^3 + 15(r-1)(4r-3)x^{4r-3}y^5\\ &+ 4\sum_{k=0}^{\frac{r-4}{2}}(7+4k)(4(r-k)-5)x^{4(r-k)-5}y^{7+4k},\end{aligned}$$

$$\begin{aligned}D_xSMP(H;x,\frac{1}{x}) &= 8(4r-4)x^{4r-4} + 3(r-1)(4r-8)x^{4r-8}\\ &+ 4\sum_{k=0}^{\frac{r-4}{2}}(4r-8k-12)x^{4r-8k-12},\end{aligned}$$

$$D_xSMP(H;x,x) = 8(4r+2)x^{4r+2} + 3(r-1)(4r+2)x^{4r+2} + 4\sum_{k=0}^{\frac{r-4}{2}}(4r+2)x^{4r+2}.$$

Then due to Table 1, we conclude that

- $Sz(H) = D_xD_ySMP(H;x,y)|_{x=y=1} = \frac{1}{3}(16r^3 + 204r^2 - 157r + 99)$,
- $PI(H) = D_xSMP(H;x,x)|_{x=1} = (5r+1)(4r+2)$,

- $Mo(H) = D_x SMP(H; x, \frac{1}{x})|_{x=1} = 16r^2 - 20r + 8.$

□

Theorem 2.3. *Let H when r is odd, $r \geq 5$. Then, its SMP-polynomial is as follows:*

$$SMP(H;x,y) = 8x^{4r-1}y^3 + 3(r-1)x^{4r-3}y^5 + 2x^{2r+1}y^{2r+1} + 4\sum_{k=0}^{\frac{r-5}{2}} x^{4(r-k)-5}y^{7+4k}.$$

Proof. By using Figure 2 and Table 3, the SMP-polynomial of H is computed as follows:

$$\begin{aligned} SMP(H;x,y) &= \sum_{e=uv\in E(G), n_u(e)\geq n_v(e)} x^{n_u(e|G)}y^{n_v(e|G)} \\ &= |E_{\{4r-1,3\}}|x^{4r-1}y^3| + |E_{\{4r-3,5\}}|x^{4r-3}y^5 + E_{\{2r+1,2r+1\}}|x^{2r+1}y^{2r+1} \\ &+ |E_{\{4r-5,7\}}|x^{4r-5}y^7 + \ldots + |E_{\{2r+5,2r-3\}}|x^{2r+5}y^{2r-3} = 8x^{4r-1}y^3 \\ &+ 3(r-1)x^{4r-3}y^5 + 2x^{2r+1}y^{2r+1} + 4x^{4r-5}y^7 + \ldots + 4x^{2r+5}y^{2r-3} \\ &= 8x^{4r-1}y^3 + 3(r-1)x^{4r-3}y^5 + 2x^{2r+1}y^{2r+1} + 4\sum_{k=0}^{\frac{r-5}{2}} x^{4(r-k)-5}y^{7+4k}. \end{aligned}$$

□

Proposition 2.4. *Consider H, when r is odd. Then the following holds:*

- $Sz(H) = \frac{1}{3}(40r^3 - 60r^2 + 779r - 981),$
- $PI(H) = (5r+1)(4r+2),$
- $Mo(H) = 16r^2 - 20r + 4.$

Proof. Let $SMP(H;x,y) = 8x^{4r-1}y^3 + 3(r-1)x^{4r-3}y^5 + 2x^{2r+1}y^{2r+1} + 4\sum_{k=0}^{\frac{r-5}{2}} x^{4(r-k)-5}y^{7+4k}$. The following results are obtained by applying the operators on the SMP-polynomial.

$$\begin{aligned} D_xD_y(SMP(H;x,y) &= 24(4r-1)x^{4r-1}y^3 + 15(4r-3)(r-1)x^{4r-3}y^5 \\ &+ 2(2r+1)^2x^{2r+1}y^{2r+1} + 4\sum_{k=0}^{\frac{r-5}{2}} \\ &(7+4k)(4(r-k)-5)x^{4(r-k)-5}y^{7+4k}, \end{aligned}$$

$$\begin{aligned} D_xSMP(H;x,\frac{1}{x}) &= 8(4r-4)x^{4r-4} + 3(r-1)(4r-8)x^{4r-8} \\ &+ 4\sum_{k=0}^{\frac{r-5}{2}}(4r-8k-12)x^{4r-8k-12}, \end{aligned}$$

$$D_xSMP(H;x,x) = 8(4r+2)x^{4r+2} + 3(r-1)(4r+2)x^{4r+2} + 2(4r+2)x^{4r+2} + 4\sum_{k=0}^{\frac{r-5}{2}}(4r+2)x^{4r+2},$$

Then due to Table 1, we conclude that

- $Sz(H) = D_xD_y(SMP(H;x,y)|_{x=y=1} = \frac{1}{3}(40r^3 - 60r^2 + 779r - 981)$,
- $PI(H) = D_xSMP(H;x,x)|_{x=1} = (5r+1)(4r+2)$,
- $Mo(H) = D_xSMP(H;x,\frac{1}{x})|_{x=1} = 16r^2 - 20r + 4$.

□

2.1 Numerical and Graphical Representation

Table 4 includes the results obtained. As the value of r increases, the values of all the indices also increase; see Figure 3. According to calculations, the Mo index, with two different formulas for the number of even and odd rings, follows a similar increasing trend, and its plot is lower than other indices. For $r \leq 12$, the Sz index for odd rings is smaller than the Sz index for even rings. However, for $r > 12$, this trend reverses. The graphic representation of this index shows that the plot of the Sz index based on odd values is higher than the plot of the same index for even values. In general, the plot of the Sz index is higher than the plots of the other discussed indices; see Figure 3.

Table 4. Numerical comparison of $PI(H)$, $Mo(H)$, and $S(H)$.

r	5	6	7	8	9	10	11	12	13	14	15	16
$PI(H)_r$	572	806	1080	1394	1748	2142	2576	3050	3510	4118	4712	5346
$Sz(H)_{r:odd}$	2138	-	5084	-	10110	-	17856	-	28962	-	44068	-
$Sz(H)_{r:even}$	-	3319	-	6697	-	11643	-	18413	-	27263	-	38449
$Mo(H)_{r:odd}$	304	-	648	-	1120	-	1720	-	2448	-	3304	-
$Mo(H)_{r:even}$	-	464	-	872	-	1408	-	2072	-	2864	-	3784

2.2 Application

In this section, it is discussed how to use Mo, Sz, and PI indices to predict some physicochemical characteristics of helicenes, see Figure 2.

The molecular weight (MW) helps determine the chemical structure and reactivity of substances. For this reason, it is an important feature in chemistry. By determining macromolecules, molecular weight affects their behavior in reactions and helps determine the con-

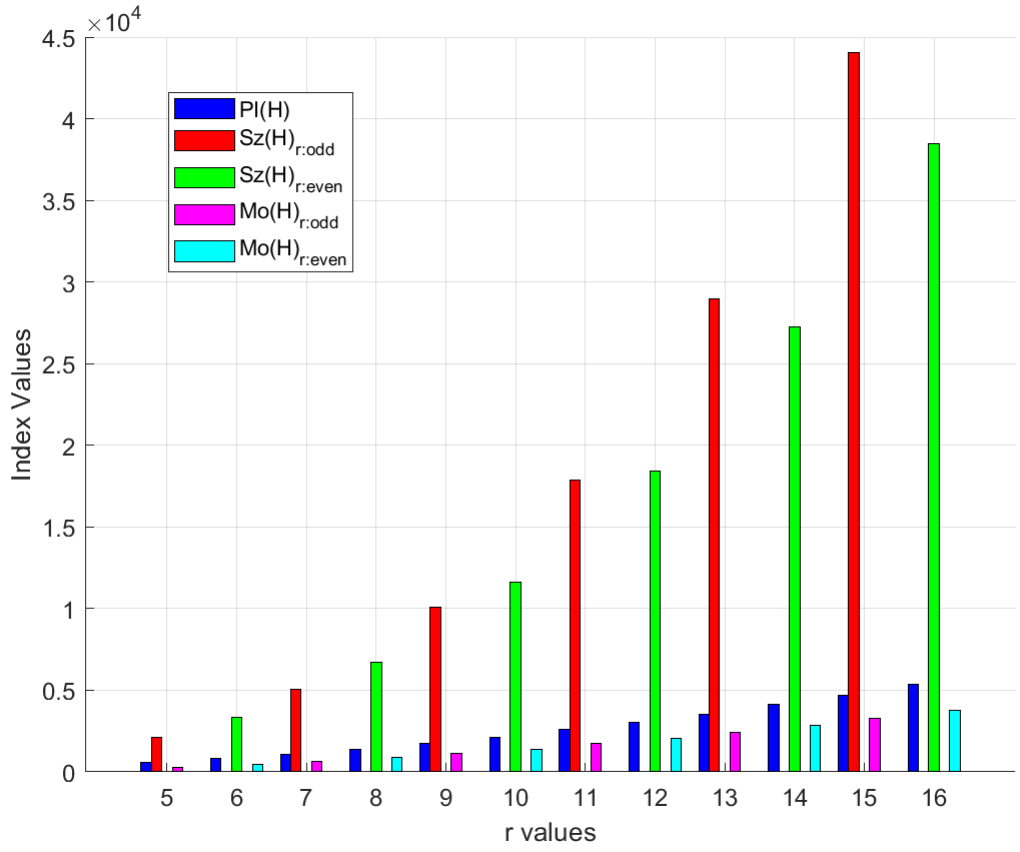

Figure 3. Comparison of the indices PI(H), Sz(H), and Mo(H) as a function of r.

centration, stoichiometry, and physical properties of substances, thereby affecting their use in various chemical formulations and processes [17].

Because factors such as gravity, impurities, and the size and structure of molecules affect the melting point (MP) of a substance, therefore, determining the melting point helps to understand the physicochemical properties. So the melting point can be used to identify a substance [18].

The heavy atom count (HAC) of a molecule is the total number of nonhydrogen atoms within the chemical structure. Heavy atomic count refers to the number of heavy atoms present in a molecular structure, particularly in crystallography and nuclear physics. Due to the importance of these characteristics, MW, MP, boiling point (BP), and HAC have been selected for the comparison testing. Also, some Helicines were chosen as test molecules for which experimental evidence exists regarding the properties we assessed, as shown in Table 5. The data for these physicochemical parameters shown in Table 5 was obtained from PubChem and ChemSpider. Table 4 includes the measured values of Mo, Sz, and PI indices for selected *H*s.

The values of the correlation coefficients between the defined topological index and the physicochemical properties of three helicenes are presented in Table 6. As shown in Table

6, the Mo index demonstrates the strongest positive correlation ($r = 0.9992$) with both MW and HAC among all the correlations. Additionally, Table 6 highlights that the Mo index is the most effective for predicting MW, BP, and HAC. However, the Mo index shows less reliability for other properties, such as MP. The Sz index also has conditions similar to the Mo index. The PI index is not very reliable for all characteristics.

Table 5. physicochemical properties of H.

Helicenes	MW	MP	BP	HAC
$[5]Helicene$	278.35	145	524.7	22
$[6]Helicene$	328.41	263	604	26
$[7]Helicene$	378.46	254	677	30

Table 6. The correlation between PI, Sz, Mo, and physicochemical properties of H.

Indices	MW	MP	PB	HAC
PI	0.2961	0.2381	0.1308	0.2961
Sz	0.9935	0.7609	0.9905	0.9935
Mo	0.9992	0.8066	0.9979	0.9992

3 Conclusions

In this paper, closed formulas for the Sz, Mo, and PI indices of the helicenes were computed with the number of even and odd rings. Calculating the topological indices via these formulas does not need to edge partitioning. They can be calculated with the number of benzene rings. As the number of benzene rings increased all indices were ascending. PI index for odd and even numbers of benzene rings were obtained from a similar formula. The Mo index with different formulas for the number of even and odd rings followed a similar increasing trend, and its plot was lower than the other plot of indices. For $r \geq 13$, the Sz index plot with the odd number of rings was higher than the other plot of indices. The topological indices are useful for understanding physical properties, biological processes, and chemical activity. The obtained results were displayed graphically and numerically. Considering that there is no need to count edges and polynomial calculations to calculate topological indices, calculations are reduced, and these results can be used in future studies. By correlation analysis between indices and physicochemical properties, the Mo index has the strongest positive correlation than other indices with physicochemical properties.

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Data Availability Statement

Data is contained within the article.

Conflicts of Interests

The authors declare that they have no competing interests.

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