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SMP-Polynomial and Topological Indices of Phenacenes

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Abstract

Phenacenes are a group of organic compounds that consist of fused aromatic rings. They also follow the general molecular formula $C_{4n+2}H_{2n+4}$. In this article, we compute the SMP polynomial for phenacenes with even and odd numbers of rings. Then, through these polynomials, we obtain general formulas for topological indices based on distances such as Sz, PI, and Mo. Using these formulas does not require counting the edges, and these indices are calculated according to the number of benzene rings in phenacenes. We display the obtained results numerically and graphically and compare topological indices graphically.

Keywords: SMP-polynomial, Szeged index, Mostar index, PI index, Phenacenes.
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1 Introduction

Phenacenes (Phas) are a group of organic compounds that consist of fused aromatic rings. They are polycyclic aromatic hydrocarbons related to acenes and helicenes that differ from them in the arrangement of fused rings. [n]Phas, the isomeric form of [n]acene, is known as a stable compound in which the benzene rings are fused in a zigzag structure and has the general formula $C_{4n+2}H_{2n+4}$, Figure 1. Molecules of this family are used for new materials due to their electronic, thermodynamic and optical properties such as superconducting, semiconducting, photoconducting, and ferromagnetic properties [[1, 2, 3, 4, 5]]. Although computational quantum chemistry has made significant progress in recent decades, topics such as band gap, electronic structure, stability and aromaticity in polyacenes are still discussed. Considering that there is no direct experimental evidence in the mentioned fields, the questions related to the electronic properties of polyacenes are of interest to physicists and quantum chemists [2]. Investigating the stability and electronic properties of polyacenes paves the way for its applications in optoelectronic and magnetic devices [3]. In chemical graphs, atoms and bonds are shown by vertices and edges, respectively. Mathematical chemistry includes tools such as polynomials, which can be calculated using mathematical models based on polynomial

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of chemical structures, predicted their physical and chemical properties. Such as M-polynomials, MN-polynomials, and SMP-polynomials. Using these polynomials, different topological indices can be obtained more easily and quickly. In 2023, Knor and Tratnik introduced SMP-polynomial. We can use this polynomial to calculate all three vertex indices Sz, Mo and PI [6]. The SMP polynomial is a new alternative to the Szeged (Sz), Mostar (Mo), and PI polynomials that has two variables and can be easily used to calculate three topological indices the Sz index, the Mo index, and the PI index of a given graph. Notice that the advantage of the introduced polynomial is that to calculate the three known molecular descriptors, only one polynomial should be considered instead of three [7]. The SMP-polynomial of G is written as

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

where $n_u(e|G) = |N_u(e|G)|$ and $N_u(e|G) = \{x \in V(G) | d_G(x,u) < d_G(x,v)\}$ are number and set of vertices of G lying closer to u, respectively, see also [8]. The Hosoya polynomial is a remarkable polynomial in the field of distance-based topological indices. S. Hameed et al. calculated the degree-based indices of Bismuth Tri-iodide structure via M-polynomial [9].

Topological indices of a graph are numerical parameters that predict the properties of the chemical graph G. They are used for in codify information regarding shape, molecular size, branching, etc [4, 5]. The oldest topological index was introduced by Harold Wiener and called the Wiener index, The Wiener index W(G) is as $W(G) = \sum_{u,v\in V(G)} d_G(u,v)$. Notice that where G is a connected graph. $d_G(u,v)$ represents the shortest path distance between vertices u and v. The Wiener index for tree T can be calculated as

$$W(T) = \sum_{e=uv\in E(T)} n_u(e|T) n_v(e|T). \tag{1}$$

where $n_u(e|T)$ signify the number of vertices of T whose distance to u is smaller than the distance to v. Similarly, we define $n_v(e|T)$. In 1994, Gutman introduced the Sz index using (1) [6]. Khadikar introduce topological index Padmakar-Ivan index and it denoted as PI, where the number of edges of G that are closer to u than v and the number of edges of G that are closer to v than u are shown by $m_u(G)$ and $m_v(G)$ respectively It will be given. Edges that are the same distance from the two end vertices of edge uv are not counted. The vertices version of this index was introduced by Ashrafi and is displayed as PI_v and it is called the PI vertex index. The Vertex PI polynomial is defined as PI_v where $n_u(e|G)$ and $n_v(e|G)$ are the number of vertices of G lying closer to u and v, respectively. Another introduced invariant of the same kind is the Sz index invented by Ivan Gutman. Mathematical properties of Sz were established and its chemical applications were reported [8]. A. Modabish et al. conducted research on diphenylene and its properties to advance new materials and technologies, particularly in the field of catalysis [10]. M. S, Sardar et al. computed topological indices for a double Graph of Alkanes using graph operations [11]. The Sz index is the oldest topological index based on distance [8, 12] and is as

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

The Mo used as a measure of peripherality in chemical graphs, is defined as [13]

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

vertex-PI index was introduced by Khadikar [8] as

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

Table 1: Derivation of some topological indices 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	$D_x(SMP(G;x,x))\|_{x=1}$

These topological indices can be calculated using SMP- polynomial and Table 1. This article gives the formula for them in terms of the number of rings.

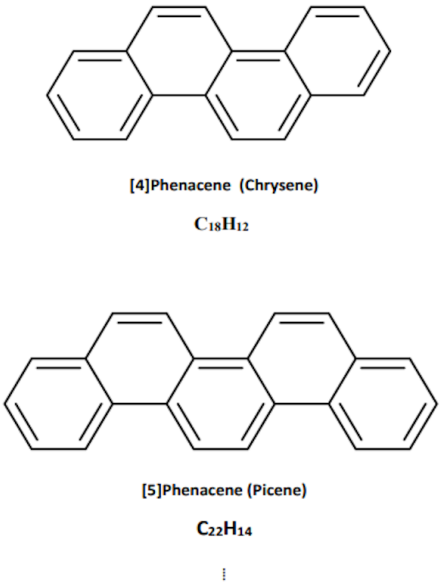

Figure 1: Phenacene(Zigzag structure).

2 Main results

Some symbols that are retained throughout the paper are explained. Let G be a simple molecular graph with no directed edges and loop-free. The number of vertices, edges, units, and benzene rings are shown by p, m, n, and r, respectively. Suppose that G is a connected graph with at least one edge.

Theorem 2.1. *Consider phenacenes with an even number of benzene rings. Then, its SMP polynomial is as follows*

$$SMP(Pha;x,y) = 3x^{2r+1}y^{2r+1} + 8x^{4r-1}y^3 + 4\sum_{k=1}^{\frac{r}{2}-1} x^{2r+4k-1}y^{2r-4k+3} + 6\sum_{k=1}^{\frac{r}{2}-1} x^{2r+4k+1}y^{2r-4k+1}$$

Table 2: Edge partition of Pha, when r is even.

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

Table 3: Edge partition of Pha, when r is odd.

(n_u, n_v)	Number of edges
(4p+3,4p+3)	2
(8p+3,3)	8
(4(p+k)+3,4(p-k)+3)	4(p-1)
(4(p+k)+1,4(p-k)+5)	6p
Total edges	10p+6
$r=2p+1,\ p\geq 1,\ 1\leq k\leq p.$	

Proof. We can calculate the SMP-polynomial of phenacenes using Figure 1 and Table 2 as follows

$$\begin{aligned}SMP(Pha;x,y) &= \sum_{n_u(e)\geq n_v(e)} x^{n_u(e|G)}y^{n_v(e|G)} = |E_{\{2r+1,2r+1\}}|x^{2r+1}y^{2r+1} + |E_{\{4r-1,3\}}|x^{4r-1}y^3\\ &+ |E_{\{2r+3,2r-1\}}|x^{2r+3}y^{2r-1} + \ldots + |E_{\{4r-5,7\}}|x^{4r-5}y^7 + |E_{\{2r+5,2r-3\}}|x^{2r+5}y^{2r-3}\\ &+ \ldots + |E_{\{4r-3,5\}}|x^{4r-3}y^5 = 3x^{2r+1}y^{2r+1} + 8x^{4r-1}y^3 + (4x^{2r+3}y^{2r-1} + \ldots + 4x^{4r-5}y^7)\\ &+ (6x^{2r+5}y^{2r-3} + \ldots + 6x^{4r-3}y^5) = 3x^{2r+1}y^{2r+1} + 8x^{4r-1}y^3 + 4\sum_{k=1}^{\frac{r}{2}-1} x^{2r+4k-1}y^{2r-4k+3}\\ &+ 6\sum_{k=1}^{\frac{r}{2}-1} x^{2r+4k+1}y^{2r-4k+1}.\end{aligned}$$

□

Proposition 2.2. *We consider the structure of Pha, with an even number of benzene rings.*

(i) Sz index: $Sz(Pha) = D_xD_y(SMP(Pha;x,y)|_{x=y=1} = \frac{1}{3}(40r^3+60r^2+107r-45)$.

(iii) PI index: $PI(Pha) = D_x(SMP(pha;x,x))|_{x=1} = (5r+1)(4r+2)$.

(ii) Mo index: $Mo(Pha) = D_x(SMP(Pha;x,\frac{1}{x}))|_{x=1} = 10r^2+4r-16$.

Proof. Let

$$SMP(Pha;x,y) = 3x^{2r+1}y^{2r+1} + 8x^{4r-1}y^3 + 4\sum_{k=1}^{\frac{r}{2}-1} x^{2r+4k-1}y^{2r-4k+3} + 6\sum_{k=1}^{\frac{r}{2}-1} x^{2r+4k+1}y^{2r-4k+1}.$$

Now, we use the formulas from Table 1, and calculate these results.

$$\begin{aligned}D_ySMP(Pha;x,y)) &= 3(2r+1)x^{2r+1}y^{2r+1} + 8(3)x^{4r-1}y^3 + 4\textstyle\sum_{k=1}^{\frac{r}{2}-1}(2r-4k+3)\\ &\quad x^{2r+4k-1}y^{2r-4k+3} + 6\textstyle\sum_{k=1}^{\frac{r}{2}-1}(2r-4k+1)x^{2r+4k+1}y^{2r-4k+1},\end{aligned}$$

$$\begin{aligned} D_x(D_y(SMP(Pha;x,y)) &= 3(2r+1)(2r+1)x^{2r+1}y^{2r+1} + 8(3)(4r-1)x^{4r-1}y^3 \\ &+4\textstyle\sum_{k=1}^{\frac{r}{2}-1}(2r-4k+3)(2r+4k-1)x^{2r+4k-1}y^{2r-4k+3} \\ &+6\textstyle\sum_{k=1}^{\frac{r}{2}-1}(2r-4k+1)(2r+4k+1)x^{2r+4k+1}y^{2r-4k+1}, \end{aligned}$$

$$D_x(SMP(Pha;x,\frac{1}{x})) = 8(4r-4)x^{4r-4} + 4\textstyle\sum_{k=1}^{\frac{r}{2}-1}(8k-4)x^{8k-4} + 6\sum_{k=1}^{\frac{r}{2}-1}(8k)x^{8k},$$

$$\begin{aligned} D_x(SMP(Pha;x,x)) &= 3(4r+2)x^{4r+2} + 8(4r+2)x^{4r+2}y^3 + 4\textstyle\sum_{k=1}^{\frac{r}{2}-1}(4r+2)x^{4r+2} \\ &+6\textstyle\sum_{k=1}^{\frac{r}{2}-1}(4r+2)x^{4r+2}, \end{aligned}$$

(i) Sz index: $Sz(Pha) = \frac{1}{3}(40r^3 + 60r^2 + 107r - 45)$.

(iii) PI index: $PI(Pha) = (5r+1)(4r+2)$.

(ii) Mo index: $Mo(Pha) = 10r^2 + 4r - 16$.

□

Theorem 2.3. *Consider phenacenes with an odd number of benzene rings. Then, its SMP-polynomial is as follows*

$$\begin{aligned} SMP(Pha;x,y) = 2x^{2r+1}y^{2r+1} + 8x^{4r-1}y^3 + 4\sum_{k=1}^{\frac{r-3}{2}} x^{2r+4k+1}y^{2r-4k+1} \\ + 6\sum_{k=1}^{\frac{r-1}{2}} x^{2r+4k-1}y^{2r-4k+3} \end{aligned}$$

Proof. We can compute the SMP-polynomial of chemical structure of phenacene using Figure 1 and Table 3 as follows

$$\begin{aligned} SMP(Pha;x,y) = \sum_{e=uv\in E(G), n_u(e)\geq n_v(e)} x^{n_u(e|G)}y^{n_v(e|G)} = |E_{\{2r+1,2r+1\}}|x^{2r+1}y^{2r+1} + |E_{\{4r-1,3\}}|x^{4r-1}y^3 \\ + |E_{\{2r+5,2r-3\}}|x^{2r+5}y^{2r-3} + \ldots + |E_{\{4r-5,7\}}|x^{4r-5}y^7 + |E_{\{2r+3,2r-1\}}|x^{2r+3}y^{2r-1} + \ldots \\ + |E_{\{4r-3,5\}}|x^{4r-3}y^5 = 2x^{2r+1}y^{2r+1} + 8x^{4r-1}y^3 + (4x^{2r+5}y^{2r-3} + \ldots + 4x^{4r-5}y^7) \\ + (6x^{2r+3}y^{2r-1} + \ldots + 6x^{4r-3}y^5) = 2x^{2r+1}y^{2r+1} + 8x^{4r-1}y^3 + 4\sum_{k=1}^{\frac{r-3}{2}} x^{2r+4k+1}y^{2r-4k+1} \\ + 6\sum_{k=1}^{\frac{r-1}{2}} x^{2r+4k-1}y^{2r-4k+3}. \end{aligned}$$

□

Proposition 2.4. *We consider the structure of Pha, with an odd number of benzene rings.*

(i) Sz index: $Sz(Pha) = D_xD_y(SMP(Pha;x,y)|_{x=y=1} = \frac{1}{3}(40r^3 + 60r^2 + 107r - 45)$,

(iii) Padmakar-Ivan (PI) index: $PI(Pha) = D_x(SMP(pha;x,x))|_{x=1} = (5r+1)(4r+2)$,

(ii) Mo index: $Mo(Pha) = D_x(SMP(Pha; x, \frac{1}{x}))|_{x=1} = 10r^2 + 4r - 14.$

Proof. Let

$$SMP(Pha; x, y) = 2x^{2r+1}y^{2r+1} + 8x^{4r-1}y^3 + 4\sum_{k=1}^{\frac{r-3}{2}} x^{2r+4k+1}y^{2r-4k+1} + 6\sum_{k=1}^{\frac{r-1}{2}} x^{2r+4k-1}y^{2r-4k+3}.$$

Then, we use from Table 1, and calculate these results.

$$\begin{aligned} D_y(SMP(Pha; x, y)) = 2(2r+1)x^{2r+1}y^{2r+1} + 24x^{4r-1}y^3 + 4\sum_{k=1}^{\frac{r-3}{2}}(2r-4k+1) \\ x^{2r+4k+1}y^{2r-4k+1} + 6\sum_{k=1}^{\frac{r-1}{2}}(2r-4k+3)x^{2r+4k-1}y^{2r-4k+3}, \end{aligned}$$

$$\begin{aligned} D_x(D_y(SMP(Pha; x, y)) = 2(2r+1)^2x^{2r+1}y^{2r+1} + 24(4r-1)x^{4r-1}y^3 \\ + 4\sum_{k=1}^{\frac{r-3}{2}}(2r-4k+1)(2r+4k+1)x^{2r+4k+1}y^{2r-4k+1} \\ + 6\sum_{k=1}^{\frac{r-1}{2}}(2r-4k+3)(2r+4k-1)x^{2r+4k-1}y^{2r-4k+3}, \end{aligned}$$

$$D_x(SMP(Pha; x, \frac{1}{x})) = 8(4r-4)x^{4r-4} + 32\sum_{k=1}^{\frac{r-3}{2}} kx^{8k} + 6\sum_{k=1}^{\frac{r-1}{2}}(8k-4)x^{8k-4},$$

$$\begin{aligned} D_x(SMP(Pha; x, x)) \quad &= 2(4r+2)x^{4r+2} + 8(4r+2)x^{4r+2} + 4\textstyle\sum_{k=1}^{\frac{r-3}{2}}(4r+2)x^{4r+2} \\ &\quad +6\textstyle\sum_{k=1}^{\frac{r-1}{2}}(4r+2)x^{4r+2}, \end{aligned}$$

(i) Sz index: $Sz(Pha) = \frac{1}{3}(40r^3 + 60r^2 + 107r - 45)$,

(iii) PI index: $PI(Pha) = (5r+1)(4r+2)$,

(ii) Mo index: $Mo(Pha) = 10r^2 + 4r - 14$.

□

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

r	2	3	4	5	6	7	8	9	10
$PI(Phas)$	110	224	378	572	806	1080	1394	1748	2142
$Sz(Phas)$	243	632	1301	2330	3799	5788	8377	11646	15675
$Mo(Phas)_{r:odd}$	-	88	-	256	-	504	-	832	-
$Mo(Phas)_{r:even}$	32	-	160	-	368	-	656	-	1024

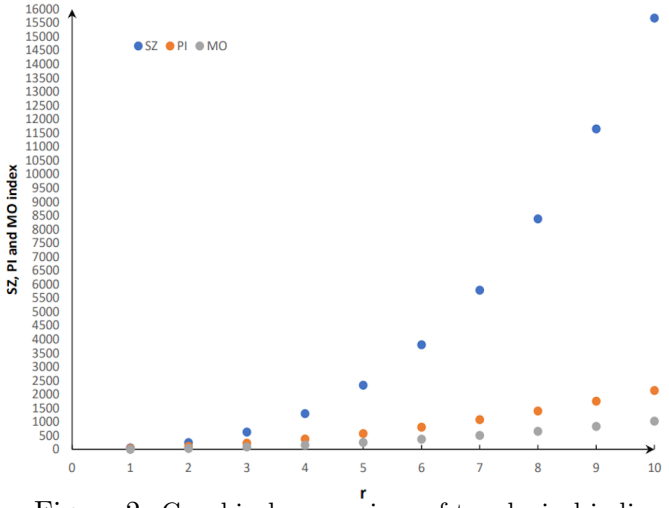

Figure 2: Graphical comparison of topological indices.

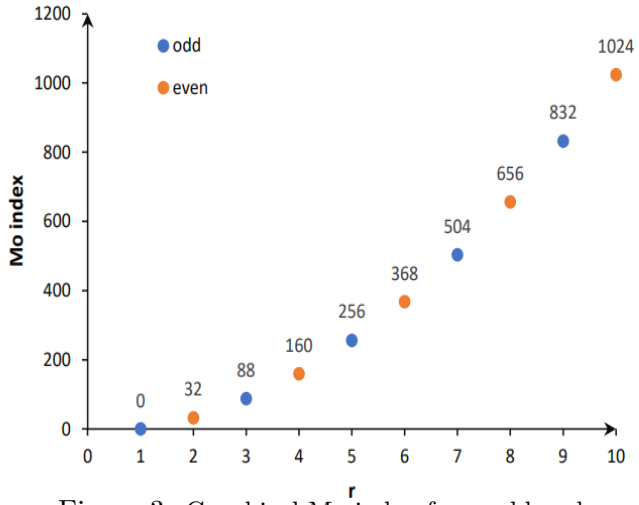

Figure 3: Graphical Mo index for r odd and even.

The obtained results are given in Table 4. The plot of these indices is in Figure 2. All of them are in ascending. Therefore, the increasing trend shows that the topological index values increase accordingly in Table 4. According to the calculations, the values of SZ and PI indices for Phas Zigzag structure with even and odd numbers of benzene rings are obtained from a similar formula. The graphical representation of the indices shows that their charts match, Figure 2. The value of the Mo index for Phas Zigzag structure with the number of even and odd rings with different formulas has a graphical display according to Figure 3.

3 Conclusion

In this article, Closed formulas of distance-dependent topological indices such as the Sz index, Mo index, and PI index of Phas Zigzag structure of Phas. These formulas are independent of counting edges. The obtained results were displayed graphically and numerically. These results can be used for the next studies because counting edges and polynomial calculations are not needed.

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