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Research Paper

Mostar index of the line graph of [n]circulenes and its comparision with the original graphs

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Abstract. In this paper, the Mostar index for $[n]$circulenes line graphs is investigated, extending previous work on the topic. This study aims to analyze the difference in the Mostar index between circulenes and their line graphs. The results show that the line graphs exhibit a higher Mostar index compared to the circulenes, with the difference growing quadratically as n increases. The derived formulas depend solely on the size of the circulene (n), simplifying the calculations. Numerical and graphical comparisons validate these results, highlighting the role of features such as cycles and degree distribution in distance-based topological indices. These findings can contribute to a better understanding of the structural properties of molecules and complex graphs.

Keywords. molecular graph, [n]circulenes, line graph, SMP-polynomial, mostar index.
Mathematics Subject Classification (2020): 05C31,05C92,05C09,05C30,05C90.

1 Introduction

$[n]$Circulenes are a class of polycyclic aromatic hydrocarbons, consisting of a central polygon surrounded by n fused benzene rings. These molecules exhibit a symmetric, disk-like geometry and, due to their unique aromaticity, electronic, optical properties, and chiroptical behavior, they have garnered attention for applications in nanophotonics, hydrogen storage, etc [1–5]. Chemical graph theory is the branch of mathematics that models molecular struc-

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tures using graph theory, where atoms are represented by vertices and chemical bonds by edges. Topological indices (TIs) are numerical descriptors derived from these graphs that are widely used to predict physicochemical and biological properties of chemical compounds [6]. TIs are contingent upon factors such as the degree of vertices and the distance between pairs of vertices [7–9]. This study aims to compute and analyze the Mostar (Mo) index of the line graph of $[n]$circulenes using the SMP-polynomial, and to compare the results with the Mo-index of the $[n]$circulene graphs. Among distance-based indices, the Mo-index is particularly notable for quantifying structural asymmetry. It is defined as [10]:

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

where $n_u(e|G)$ is the number of vertices closer to u than to v. This index captures structural imbalance by evaluating the difference in neighborhood size across each edge. In the context of line graphs, where edges of the original molecular graph are represented as vertices, the Mo-index offers a distinct perspective, potentially revealing hidden structural features related to molecular stability and reactivity [11–13]. To facilitate the computation of such indices, one powerful approach involves the use of topological polynomials. These polynomials encode topological characteristics of graphs into compact mathematical expressions, enabling efficient calculation of indices. Examples include M, MN, and SMP-polynomials. In this study, the SMP-polynomial is utilized to compute the Mo-index, particularly for complex graphs such as line graphs, where traditional methods may become cumbersome. The SMP-polynomial G is defined as [14]:

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

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

In a previous study, an examination of certain distance-based TIs of the molecular graph of $[n]$circulenes was conducted [15]. Building upon that work, the present article focuses on the structural analysis of the line graph of $[n]$circulenes. These graphs represent the relationships between bonds rather than atoms. This bond-based perspective complements atom-based analysis, offering deeper insights. By transforming the edges of a molecular graph into vertices, line graphs reveal new topological features that are especially useful for analyzing molecular structure and symmetry. Applying the Mo-index to these graphs offers novel insights into structural asymmetry and molecular characteristics, particularly in circulenes. Since the Mo-index quantifies structural imbalance, it can provide valuable information about the stability and reactivity of molecules in the context of their line graphs. In 2018, Doslic et al. introduced the Mo-index and explored its extremal properties across various graph types [11]. In 2020, Ghorbani et al. determined the Mo-index of a class of patch fullerenes [16]. In 2020, Gao et al. investigated the difference between the Mo-index and the irregularity of graphs, focusing on the difference $\Delta \text{Mo}(G) = \text{Mo}(G) - \text{irr}(G)$ for various graph classes, including trees and cactus graphs [13]. In 2021, Liu et al. introduced the edge Mo-index and studied its extremal values for trees, unicyclic graphs, and cacti [12]. In previous research, distance-based indices such as Szeged, Mo, and PI were calculated and analyzed for $[n]$circulenes structures using SMP-polynomials. This approach led to simple formulas that depend on the size of the central polygon, which facilitated the calculation of the indices without the need for edge partitioning. [15]. Continuing that research, the present paper investigates the Mo-index in line graphs corresponding to $[n]$circulenes. In this regard, using the same SMP-polynomial-based method, the Mo-index for the line graph $L(G)$ is obtained and compared with the Mo-index of the original graph G. This comparison not only provides new information about the structural changes between the graph and the line graph, but can also be useful in the analysis of molecular properties such as stability and reactivity. While in 2023, Sardar et al. proved that the Mo-index of the line graph of any tree is less than the tree itself, i.e., $\text{Mo}(L(T_n)) < \text{Mo}(T_n)$, which has been confirmed both theoretically and computationally [17].

In this study, however, we focus on graphs with cycles, in particular line graphs of circulenes. This shift in focus is especially important for understanding how transforming cyclic structures into their line graph counterparts affects their topological properties, particularly the Mo-index, and provides new insights into the molecular symmetry and reactivity of circulenes. The Mo-index of the line graph of $[n]$circulenes is computed using the SMP-polynomial and compared with that of the original circulenes graphs. The next section presents the detailed computations, formulas, and comparison of the results, highlighting the structural differences and their implications for molecular properties.

2 Results and Discussion

In this section, let C_n be the molecular graph of $[n]$circulenes, as shown in Figure 1(a). The Mo-index of $[n]$circulenes, which depends on the size of the central polygon, has been previously obtained as follows [15]:

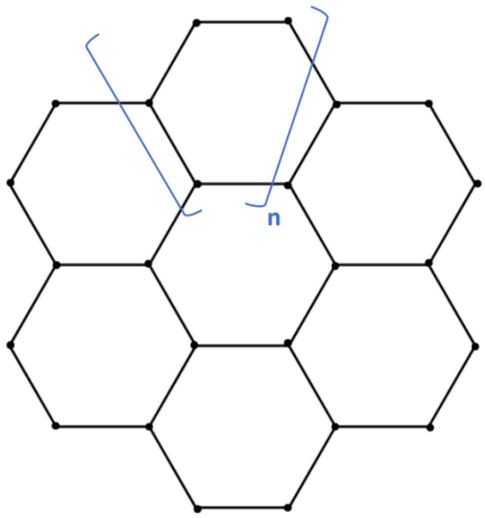
$$\text{Mo}(C_n) = 12n^2 - 30n. \quad (1)$$

Next, consider the line graph of $[n]$circulenes, denoted by $L(C_n)$, as shown in Figure 1(b). This graph has $p = 5n$ vertices and $q = 8n$ edges.

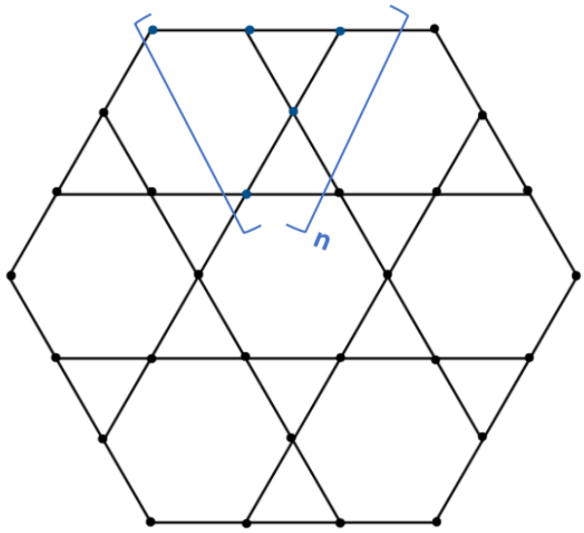
Using the same methodology based on SMP-polynomials, the Mo-index of the line graph of $[n]$circulenes is calculated. Derivation of the Mo-index from the SMP-polynomial is as follows [7]:

$$\text{Mo}(G) = D_x(SMP(G; x, \frac{1}{x}))|_{x=1}. \quad (2)$$

The edge partitioning used in the analysis is summarized in Tables 1 and 2, which include the size of the central polygon, the classification of edge types, and their respective counts.



(a): Structure of the base graph of $[n]$circulene.



(b): Structure of the line graph of the base graph of $[n]$circulene.

Figure 1.

Type of edges	$(5n-8,3)$	$(\frac{5n-2}{2},5)$	$(\frac{5n+2}{2},6)$	$(\frac{5n-8}{2},\frac{5n-8}{2})$	$(5,5)$
Number of edges	$2n$	$2n$	$2n$	n	n

Table 1. Edge partition of $L(C_n)$ when n is even, where $n \geq 4$.

Theorem 2.1. *Let G be the base graph of $L(C_n)$, where $n \geq 4$. Then:*
Case 1: *When n is even, the SMP-polynomial of G is:*

$$SMP(G;x,y) = 2nx^{5n-8}y^3 + 2nx^{\frac{5n-2}{2}}y^5 + 2nx^{\frac{5n+2}{2}}y^6 + nx^{\frac{5n-8}{2}}y^{\frac{5n-8}{2}} + nx^5y^5.$$

Case 2: *When n is odd, the SMP-polynomial of G is:*

$$SMP(G;x,y) = 2nx^{5n-8}y^3 + 2nx^{\frac{5n-3}{2}}y^5 + 2nx^{\frac{5n+3}{2}}y^6 + nx^{\frac{5n-7}{2}}y^{\frac{5n-7}{2}} + nx^5y^5.$$

Proof. For the case where n is even, using Table 1, the SMP-polynomial of G is calculated as follows:

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

For the case where n is odd, using Table 2, the SMP-polynomial of G is calculated as follows:

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

Type of edges	$(5n-8,3)$	$(\frac{5n-3}{2},5)$	$(\frac{5n+3}{2},6)$	$(\frac{5n-7}{2},\frac{5n-7}{2})$	$(5,5)$
Number of edges	$2n$	$2n$	$2n$	n	n

Table 2. Edge partition of $L(C_n)$ when n is odd, where $n \geq 5$.

□

Proposition 2.2. *Let $L(C_n)$ be the line graph of $[n]$circulenes. Then the Mo-index of $L(C_n)$ is given by:*

$$\mathrm{Mo}(L(C_n)) = 20n^2 - 44n,$$

for every integer $n \geq 4$.

Proof. The Mo-index is calculated using the SMP-polynomial for two cases based on whether n is even or odd.

Case 1: n is even. The SMP-polynomial of $L(C_n)$ is:

$$SMP(L(C_n);x,y) = 2nx^{5n-8}y^3 + 2nx^{\frac{5n-2}{2}}y^5 + 2nx^{\frac{5n+2}{2}}y^6 + nx^{\frac{5n-8}{2}}y^{\frac{5n-8}{2}} + nx^5y^5.$$

The following results are obtained by applying the operator D_x according to Equation 2 on the SMP-polynomial:

$$D_xSMP(L(C_n);x,\tfrac{1}{x}) = 2n(5n-11)x^{5n-11} + n(5n-12)x^{\frac{5n-12}{2}} + n(5n-10)x^{\frac{5n-10}{2}}.$$

Evaluating at $x = 1$, the Mo-index is obtained as follows:

$$\mathrm{Mo}(L(C_n)) = 2n(5n-11) + n(5n-12) + n(5n-10) = 20n^2 - 44n.$$

Case 2: n is odd. The SMP-polynomial of $L(C_n)$ is:

$$SMP(L(C_n);x,y) = 2nx^{5n-8}y^3 + 2nx^{\frac{5n-3}{2}}y^5 + 2nx^{\frac{5n+3}{2}}y^6 + nx^{\frac{5n-7}{2}}y^{\frac{5n-7}{2}} + nx^5y^5.$$

Applying D_x according to Equation 2 and evaluating at $x = 1$:

$$D_xSMP(L(C_n);x,\tfrac{1}{x}) = 2n(5n-11)x^{5n-11} + n(5n-13)x^{\frac{5n-13}{2}} + n(5n-9)x^{\frac{5n-9}{2}},$$

$$\mathrm{Mo}(L(C_n)) = 2n(5n-11) + n(5n-13) + n(5n-9) = 20n^2 - 44n.$$

Thus, in both cases, the formula holds. □

Corollary 2.3. *Let C_n be $[n]$circulenes graph of size n. Then, for $n \geq 4$, the following relation holds:*

$$\mathrm{Mo}(L(C_n)) > Mo(C_n).$$

Proof. From Equation 1 and Proposition 2.2, the Mo indices of C_n and its line graph are given by:

$$\mathrm{Mo}(C_n) = 12n^2 - 30n, \quad Mo(L(C_n)) = 20n^2 - 44n.$$

The difference between the two indices is computed as:

$$\mathrm{Mo}(L(C_n)) - Mo(C_n) = 8n^2 - 14n = 2n(4n-7),$$

For $n \geq 4$, it follows that $8n^2 - 14n > 0$, thus:

$$\mathrm{Mo}(L(C_n)) > Mo(C_n).$$

□

The Mo-index for both the base graphs C_n and $L(C_n)$, as well as the differences between their Mo indices, were computed for values of $4 \leq n \leq 20$. These computations were based on the derived formulas as functions of n and were performed using MATLAB scripts. The code is available upon request. The results are presented in Table 3 and Figures 2 and 3. These figures clearly show that the Mo-index of $L(C_n)$ consistently exceeds that of C_n for all values of n considered. As observed in Figure 2 and Table 3, the difference in the Mo indices between $L(C_n)$ and the C_n graphs grows quadratically as n increases. To further analyze the behavior of the Mo-index, the difference between the indices of the base graph and the line graph was plotted against n in Figure 3. The quadratic nature of this growth is evident, as the difference follows the expression $\mathrm{Mo}(L(C_n)) - \mathrm{Mo}(C_n) = 2n(4n-7)$. This result highlights the accelerated growth in the Mo-index difference as n increases, emphasizing the structural impact of the transition from the base graph to its line graph. This numerical and graphical analysis effectively supports the theoretical findings and reveals the structural differences between line graphs and base graphs in the context of distance-based TIs.

n	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
$\mathrm{Mo}(C_n)$	72	150	252	378	528	702	900	1122	1368	1638	1932	2250	2592	2958	3348	3762	4200
$\mathrm{Mo}(L(C_n))$	144	280	456	672	928	1224	1560	1936	2352	2808	3304	3840	4416	5032	5688	6384	7120
$\mathrm{Mo}(L(C_n)) - \mathrm{Mo}(C_n)$	72	130	204	294	400	522	660	814	984	1170	1372	1590	1824	2074	2340	2622	2920

Table 3. Comparison of Mo-index for $[n]$circulene and its Line Graph for different values of n.

3 Conclusion

In this study, the behavior of the Mo-index in the class of $[n]$circulene graphs and their line graphs was investigated. Closed and explicit formulas for both indices *Mo* were derived, which depend only on the parameter n. These formulas reveal a dependence of the Mo-index on the graph's central polygon size, without being influenced by other structural features. It was shown that for every $n \geq 4$, the Mo-index of the line graph $\mathrm{Mo}(L(C_n))$ is greater than that of the original graph $\mathrm{Mo}(C_n)$, and their difference follows a quadratic relationship of the form $2n(4n-7)$. To validate these theoretical results, numerical and graphical analyses were performed. The Mo indices of the original and line graphs were computed for values of $4 \leq n \leq 20$ using MATLAB. As shown in Figures 2 and 3 and Table 3, the Mo-index increases regularly under the transformation to the line graph, and its difference grows quadratically

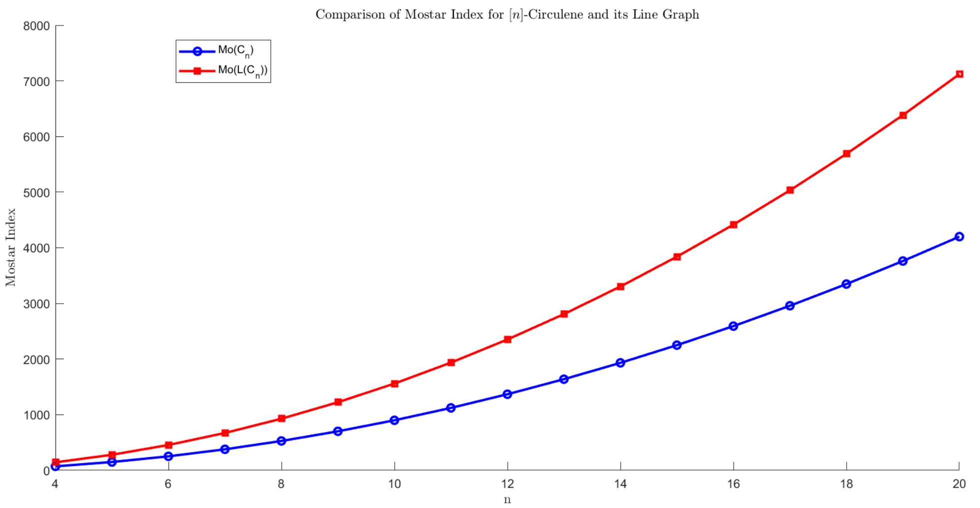


Figure 2. Comparison of Mo-index for $[n]$circulene and its Line Graph.

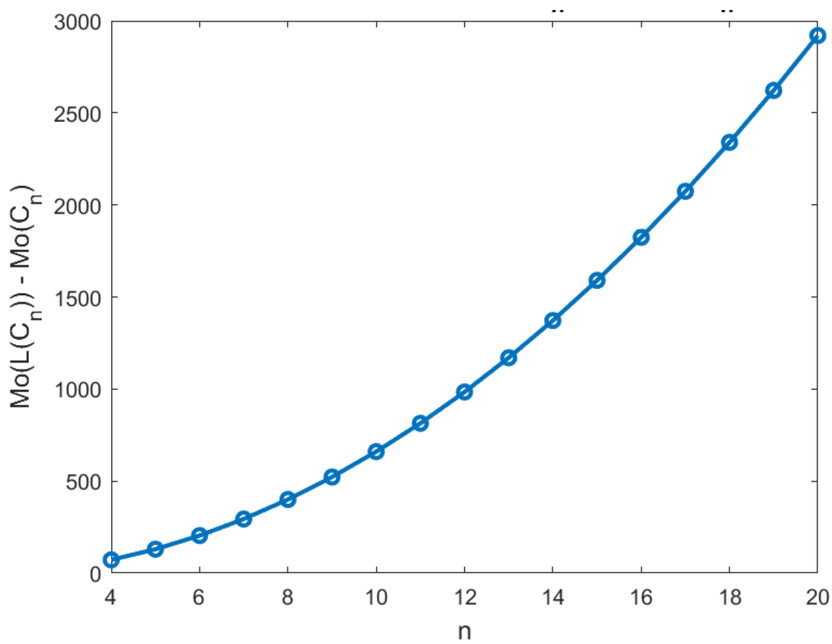


Figure 3. Difference between $\mathrm{Mo}(LC_n)$ and $\mathrm{Mo}(C_n)$.

with n. These findings highlight the structural impact of the line graph transformation, as it increases asymmetry and the distance between vertices. It is emphasized that these results specifically relate to the $[n]$circulene family. The increase in the Mo-index due to the transformation to a line graph may not hold for all cycle graphs. Previous studies on acyclic graphs, such as trees, have shown that the Mo-index decreases under this transformation. This contrast highlights the deep interplay between graph structure and distance-based TIs, emphasizing the role of features like cycles and degree distribution in shaping such metrics. It is suggested that future research explore the behavior of the Mo-index in other families of cycle graphs, especially those with irregular or complex structures, to determine whether similar patterns are observed. Such studies could deepen our understanding of the effects of graph transformations on TIs and expand their applications in fields such as mathematical chemistry and network analysis.

Finding

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Data Availability Statement

Data is contained within the article.

Conflicts of Interests

The authors declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

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