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Leap indices and their polynomials of the derived graph of the subdivision of certain polyphenyls

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Topological indices are real (numerical) values which are associated with chemical compositions to correlate with chemical structure with different physical properties, chemical and biological activities. In this article, we computed and compared leap Zagreb indices and leap hyper-Zagreb indices of the derived graph of the subdivision of certain polyphenyls based on the 2-distance degree of the vertices.

KEYWORDS

Topological indices; polyphenyls; leap Zagreb indices; subdivision; line graph.

Introduction

The graph G^* under consideration is simple and finite with V(G^*) and E(G^*) called the vertex set and the edge set, respectively. The degree d_x of any vertex x is the cardinality of vertices that are at path of length 1 from a vertex x. The shortest path between two vertices x and y of a graph G^*, represented by d(x;y), is the distance between x and y. The topological indices are used for modeling information of molecules and atoms in synthetically and structural chemistry [10-13, 16]. The subdivision graph of G^*, denoted by S(G^*), is a graph in which |E(S(G^*))|=2|E(G^*)|. The derived graph (line graph) L(G^*) of graph G^* has vertex set which is the edge set of graph G^* and 2 vertices of derived graph L(G^*) have common vertex if and only if their corresponding edges have a common vertex in G^* [1]. There more details on the derived graph of the subdivision [8, 9, 14, 15, 24, 25]. For a vertex y in G^*, the open k neighborhood of y is defined as $N_k(y/G^*)=\{u\in V(G^*):d(x,y)=k\}$, where k is a non-negative integer. The k-distance degree, denoted by $d_k(y/G^*)$, of a vertex x∈V(G^*) is the number of k neighbors of y in G^*, i:e: $d_k(y/G^*)=|N_k(y/G^*)|$. It is clear that $d_1(y/G^*)=d_y$ for every y∈V(G^*). The 2-distance degree of a vertex y is the number of vertices at distance two to y.

In a graph G^*, a vertex y is a cut vertex if its deletion increase components in G^*. An edge xy in G^* is cut-edge if its deletion along with its adjacent vertices increase components in G^*. If the cardinality of cut vertices of each hexagon in graph G^* is at most two and all cut-vertices are shared by only one hexagon and with one cut-edge, then G^* is polyphenyl hexagon(PH) chain. The length of PH chain is the number of hexagons in PH chain. The PH chain with length n has 6n vertices and 7n-1 edges. There are more details on topological indices of certain polyphenyls [4-6, 11, 25-39].

Naji et al (2017) gave explicit formulation of leap Zagreb indices of some graphs [20]. P. Shiladhar et al., calculated leap Zagreb indices of some wheel related graphs [23]. There are further properties of leap graphs [7, 3, 18-22].

The 1st, 2nd, and 3rd leap Zagreb indices for a simple graph G^* with their polynomials are as follows:

$$LM_1(G^*) = \sum_{y\in V(G^*)} (d_2(y/G^*))^2. \quad (1)$$

$$LM_2(G^*) = \sum_{xy\in E(G^*)} d_2(x/G^*)(d_2(y/G^*). \quad (2)$$

$$LM_3(G^*) = \sum_{x\in V(G^*)} d_1(x/G^*)d_2(x/G^*). \quad (3)$$

$$LM_1(G^*,r) = \sum_{xy\in E(G^*)} r^{[d(x/G^*)+d(y/G^*)]}. \quad (4)$$

$$LM_2(G^*,r) = \sum_{xy\in E(G^*)} r^{[d(x/G^*)d(y/G^*)]}. \quad (5)$$

respectively.

In 2019, leap hyper-Zagreb indices were introduced by V. R. Kulli. Leap hyper-Zagreb indices of some nanostructures and of certain windmill graphs are computed by B. Basavanagoud, E. Chitra, respectively [2] and V. R. Kulli [17].

The first and second leap hyper-Zagreb indices for a simple graph G^* with their polynomials are as follows:

$$HLM_1(G^*) = \sum_{xy\in E(G^*)})d_2(x/G^*)+d_2(y/G^*))^2. \quad (6)$$

$$HLM_2(G^*) = \sum_{xy\in E(G^*)} (d_2(x/G^*)d_2(y/G^*))^2. \quad (7)$$

$$HLM_1(G^*,r) = \sum_{xy\in E(G^*)} r^{(d(x/G^*)+d(y/G^*))^2}. \quad (8)$$

$$HLM_2(G^*,r) = \sum_{xy\in E(G^*)} r^{(d(x/G^*)d(y/G^*))^2}. \quad (9)$$

respectively.

Leap Zagreb and leap hyper-Zagreb indices of the derived graph of $S(O_n)$, $S(M_n)$ and $S(P_n)$

The subdivision graphs $S(O_n)$, $S(M_n)$ and $S(P_n)$ have 13n-1 vertices and 14n-2 edges. The graphs $L(S(O_n))$, $L(S(M_n))$ and $L(S(P_n))$ are derived graphs of $S(O_n)$, $S(M_n)$ and $S(P_n)$. In this section, we will give some explicit formulas of leap Zagreb and leap hyper-Zagreb indices of $L(S(O_n))$, $L(S(M_n))$ and $L(S(P_n))$, see Figures 1, 2, 3.

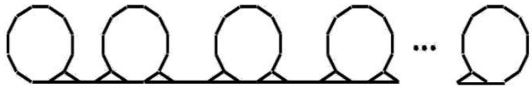

FIGURE 1 The derived graph of $S(O_n)$.

Theorem 1. If $L(S(O_n))$ is the derived graph of $S(O_n)$, then

(1) $LM_1(L(S(O_n)))=124n-72$.

(2) $LM_2(L(S(O_n)))=162n-126$.

(3) $LM_3(L(S(O_n)))=102n-56$.

(4) $HLM_1(L(S(O_n)))=654n-508$.

(5) $HLM_2(L(S(O_n)))=1914n-2142$.

Proof. Let the graph $L(S(O_n))$ in Figure 2 be the derived graph of the subdivision of meta-polyphenyl chain with $|V[L(S(O_n))]|=14n-2$ and $|E[L(S(O_n))]|=17n-5$.

For an edge $xy \in E(L(S(O_n))$, the 2-distance degree of a vertex x and vertex y is denoted by $d_2(x/L(S(O_n)))$ and $d_2(y/L(S(O_n))$, respectively. The partitioning of $E[L(S(O_n))]$ with respect to 2-distance degree of an edge xy in $E[L(S(O_n))]$ where $d_2(x/L(S(O_n)))$ $d_2(y/L(S(O_n)))\in E[L(S(O_n))]$ and the partitioning of $V[L(S(O_n))]$ depends on the 1-distance degree and 2-distance degree of a vertex x, where $d_1(x/L(S(O_n)))$, $d_2(x/L(S(O_n))\in V(L(S(O_n))$ which can be seen in Tables 1 and 2.

TABLE 1 The partition of $E(L(S(O_n)))$.

No. of edges	$d_2(x/L(S(O_n)))$	$d_2(y/L(S(O_n)))$
5n+4	*2*	*2*
2n	*2*	*3*
2(n+1)	*3*	*3*
2(2n-2)	*3*	*4*
4n-7	*4*	*4*

TABLE 2 The partition of $V(L(S(O_n)))$.

No. of edges	$d_2(x/L(S(O_n)))$	$d_2(y/L(S(O_n)))$
2(3n+2)	*2*	*2*
2n	*2*	*3*
2n	*3*	*3*
2(2n-3)	*3*	*4*

Using Formula (1) and Table 2, we have

$$LM_1(L(S(O_n))) = 2(3n+2)(2)^2 + 4n(3)^2$$
$$+2(2n-3)(4)^2 = 124n-72.$$

Using Formula (2) and Table 1, we have
$LM_2(L(S(O_n)))=(5n+4)(2.2)+2n(2.3)$
$+2(n+1)(3.3)+2(2n-2)(3.4)+(4n-7)(4.4)$
$=162n-126.$

Using Formula (3) and Table 2, we have
$LM_3(L(S(On)))=2(3n+2)(2.2)+2n(3.3)$
$+2n(2.3)+2(2n-3)(3.4)=102n-56.$

Using Formula (6) and Table 1, we have
$$HLM_1(L(S(O_n))) = (5n+4)(2+2)^2 + 2n(2+3)^2$$
$$+2(n+1)(3+3)^2 + 2(2n-2)(3+4)^2$$
$$+(4n-7)(4+4)^2 = 654n-508.$$

Using Formula (7) and Table 1, we have
$HLM_1(L(S(O_n)))=(5n+4)(2+2)^2+2n(2+3)^2$
$+2(n+1)(3+3)^2+2(2n-2)(3+4)^2$
$+(4n-7)(4+4)^2=654n-508.$
$HLM_2(L(S(O_n)))=(5n+4)(2.2)^2+2n(2.3)^2$
$+2(n+1)(3.3)^2+2(2n-2))(3.4)^2$
$+(4n-7)(4.4)^2=1914n-2142.$

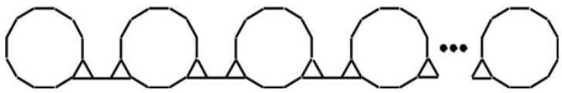

FIGURE 2 The derived graph of $S(M_n)$.

Theorem 2. If $L(S(O_n))$ is the derived graph of $S(O_n)$, then
(1)$LM_1(L(S(O_n));r)=(5n+4)r^4+2nr^5+2(n+1)r^6$
$+2(2n-2)r^7+(4n-7)r^8.$
(2)$LM_2(L(S(O_n));r)=(5n+4)r^4+2nr^6+2(n+1)r^9$
$+2(2n-2)r^{12}+(4n-7)r^{16}.$
(3)$HLM_1(L(S(O_n));r)=(5n+4)r^{16}+2nr^{25}$
$+2(n+1)r^{36}+2(2n-2)r^{49}+(4n-7)r^{64}.$
(4)$HLM_2(L(S(O_n));r)=(5n+4)r^{16}+2nr^{36}$
$+2(n+1)r^{81}+2(2n-2)r^{144}+(4n-7)r^{256}.$

Proof. Using Formulas of 4,5,8,9 and Tables 1 and 2), we have them.■

Theorem 3. If $L(S(M_n))$ is the derived graph of $S(M_n)$, then
(1)$LM_1(L(S(M_n)))=120n-72.$
(2)$LM_2(L(S(M_n)))=151n-104.$
(3)$LM_3(L(S(M_n)))=100n-52.$
(4)$HLM_1(L(S(M_n)))=50n^2+510n-420.$
(5)$HLM_2(L(S(M_n)))=72n^2+1375n-1352.$

Proof. The partitioning of $E[L(S(M_n))]$ with respect to 2-distance degree of an edge xy in $L(S(M_n))$ where $d_2(x/L(S(M_n)))$ $d_2(y/L(S(M_n)))\in E(L(S(M_n))$ and the partitioning of $V[L(S(M_n))]$ depends on the 1-distance degree and 2-distance degree of a vertex x, where $d_1(x/L(S(M_n)))$, $d_2(x/L(S(M_n)))$ $\in V(L(S(M_n)))$ which can be seen in Tables 3 and 4, respectively.

TABLE 3 The partition of $E(L(S(M_n)))$.

No. of edges	$d_2(x/L(S(M_n)))$	$d_2(y/L(S(M_n)))$
$3n+8$	2	2
$2n$	2	3
$7n-8$	3	3
$4(n-1)$	3	4
$n-1$	4	4

TABLE 4 The partitioning of $V(L(S(M_n)))$.

No. of edges	$d_1(x/L(S(M_n)))$	$d_2(y/L(S(M_n)))$
$4(n+2)$	2	2
$4(n-1)$	2	3
$4(n-1)$	3	3
$2(n-1)$	3	4

Using Formula (1) and Table 4, we have
$LM_1(L(S(M_n)))=4(n+2)(2)^2+8(n-1)(3)^2$
$+(2n-2)(4)^2=120n-72.$

Using Formula (2) and Table 3, we have
$LM_2(L(S(M_n)))=(3n+8)(2.2)+2n(2.3)$
$+(7n-8)(3.3)+4(n-1)(3.4)+(n-1)(4.4)$
$=151n-104.$

Using Formula (3) and Table 4, we have
$LM_3(L(S(M_n)))=4(n+2)(2.2)+4(n-1)(2.3)$
$+4(n-1)(3.3)+(2n-2)(3.4)=100n-52.$

Using Formula (6) and Table 3, we have
$HLM_1(L(S(M_n)))=(3n+8)(2+2)^2$

$+2n(n-1)(2+3)^2+(7n-8)(3+3)^2$
$+4(n-1)(3+4)^2+(n-1)(4+4)^2$
$=50n^2+510n-420.$

Using Formula (7) and Table 3, we have
$HLM_2(L(S(M_n)))=(3n+8)(2.2)^2$
$+2n(n-1)(2.3)^2+(7n-8)(3.3)^2+4(n-1)(3.4)^2$
$+(n-1)(4.4)^2=72n^2+1375n-1352.$

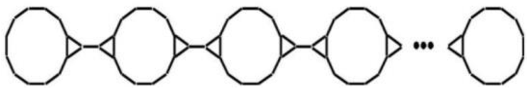

FIGURE 3 The derived graph of S(P_n).

Theorem 4. If L(S(M_n)) is the derived graph of S(M_n), then
$(1)LM_1(L(S(M_n));r)=(3n+8)r^4+2nr^5+(7n8)r^6$
$+4(n-1)r^7+(n-1)r^8$
$(2)LM_2(L(S(M_n));r)=(3n+8)r^{4+}2nr^6+(7n8)r^9$
$+4(n-1)r^{12}+(n-1)r^{16}.$
$(3)HLM_1(L(S(M_n));r)=(3n+8)r^{16}+2nr^{25}$
$+(7n-8)r^{36}+4(n-1)r^{49}+(n-1)r^{64}.$
$(4)HLM_2(L(S(M_n));r)=(3n+8)r^{16}+2nr^{36}$
$+(7n-8)r^{81}+4(n-1)r^{144}+(n-1)r^{256}.$

Proof. Using Formulas of 4,5,8,9 and Tables 3 and 4, we have them.■

Theorem 5. If L(S(P_n)) is the derived graph of S(P_n), then
$(1)LM_1[L(S(P_n))]=120n-72.$
$(2)LM_2[L(S(P_n))]=150n-102.$
$(3)LM_3[L(S(P_n))]=100n-52.$
$(4)HLM_1[L(S(P_n))]=608n-416.$
$(5)HLM_2[L(S(P_n))]=1494n-1302.$

Proof. The partitioning of E[L(S(P_n))] with respect to 2-distance degree of an edge $xy \in L(S(P_n))$ where $d_2(x/L(S(P_n)))$ $d_2(y/L(S(P_n))) \in E(L(S(P_n))$ and the partitioning of V[L(S(P_n))] depend on the 1-distance degree and 2-distance degree of a vertex x, where $d_1(x/L(S(P_n)))$, $d_2(x/L(S(P_n)))$ $\in V(L(S(P_n)))$ which can be seen in Tables 5 and 6, respectively.

Using Formula (1) and Table 6, we have
$LM_1[L(S(P_n))]=4(n+2)(2)^2+8(n-1)(3)^2$
$+(2n-2)(4)^2=120n-72.$

Using Formula (2) and Table 5, we have
$LM_2[L(S(P_n))]=2(n+5)(2.2)+4(n-1)(2.3)$
$+(6n-6)(3.3)+4(n-1)(3.4)+(n-1)(4.4)$
$=150n-102.$

TABLE 5 The partition of E(L(S(P_n))).

No. of edges	$d_2(x/L(S(P_n)))$	$d_2(y/L(S(P_n)))$
2(n+5)	2	2
4(n-1)	2	3
6(n-1)	3	3
4(n-1)	3	4
n-1	4	4

TABLE 6 The partition of V(L(S(P_n)))

No. of edges	$d_1(x/L(S(P_n)))$	$d_2(x/L(S(P_n)))$
4(n+2)	2	2
4(n-1)	2	3
4(n-1)	3	3
2(n-1)	3	4

Using Formula (3) and Table 6, we have
$LM_3[L(S(P_n))]=4(n+2)(2.2)+4(n-1)(2.3)$
$+4(n-1)(3.3)+(2n-2)(3.4)=100n-52.$

Using Formula (6) and Table 5, we have
$HLM_1[L(S(P_n))]=2(n+5)(2+2)^2+4(n-1)(2+3)^2$
$+6(n-1)(3+3)^2+4(n-1)(3+4)^2+(n-1)(4+4)^2$
$=608n-416.$

Using Formula (7) and Table 5, we have
$HLM_2[L(S(P_n))]=2(n+5)(2.2)^2+4(n-1)(2.3)^2+6(n-1)(3.3)^2+4(n-1)(3.4)^2+(n-1)(4.4)^2=1494n-1302.$

Theorem 6. Let L(S(P_n)) be the derived graph of the S(P_n), then
$(1)LM_1(L(S(P_n));r)=2(n+5)r^4+4(n-1)r^5$
$+(6n-6)r^6+4(n-1)r^7+(n-1)r^8.$
$(2)LM_2(L(S(P_n));r)=2(n+5)r^4+4(n1)r^6$
$+(6n-6)r^9+4(n-1)r^{12}+(n-1)r^{16}.$
$(3)HLM_1(L(S(P_n));r)=2(n+5)r^{16}$
$+4(n-1)r^{25}+(6n-6)r^{36}+4(n-1)r^{49}+(n-1)r^{64}.$
$(4)HLM_2(L(S(P_n));r)=2(n+5)r^{16}+4(n-1)r^{36}$
$+(6n-6)r^{81}+4(n-1)r^{144}+(n-1)r^{256}.$

Proof. Using Formulas (4,5,8,9) and Tables 5 and 6.■

Comparison of numerical values of leap Zagreb and leap hyper-Zagreb indices of the derived graphs of $S(O_n)$, $S(M_n)$ and $S(P_n)$

In this section, the numerical values of leap Zagreb and leap hyper-Zagreb indices of the derived graphs of $S(O_n)$, $S(M_n)$ and $S(P_n)$ were compared, see Figures 4-8.

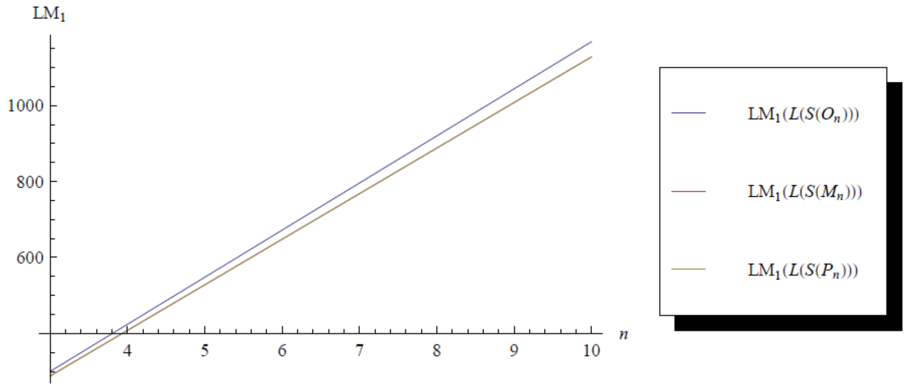

FIGURE 4 Comparison of first leap Zagreb index of the derived graphs of $S(O_n)$, $S(M_n)$ and $S(P_n)$.

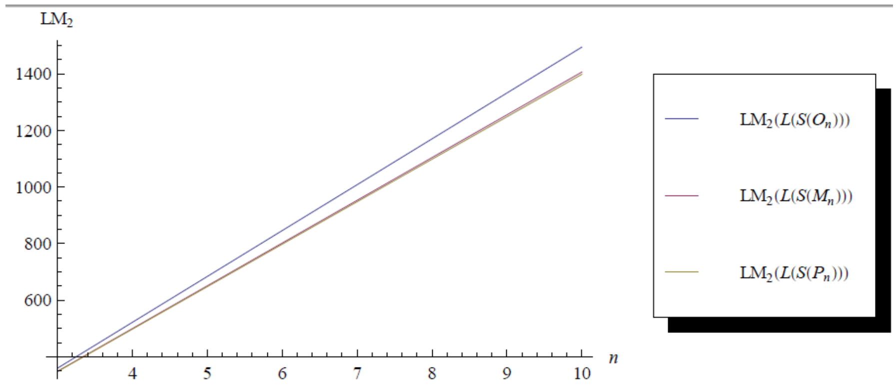

FIGURE 5 Comparison of second leap Zagreb index of the derived graphs of $S(O_n)$, $S(M_n)$ and $S(P_n)$

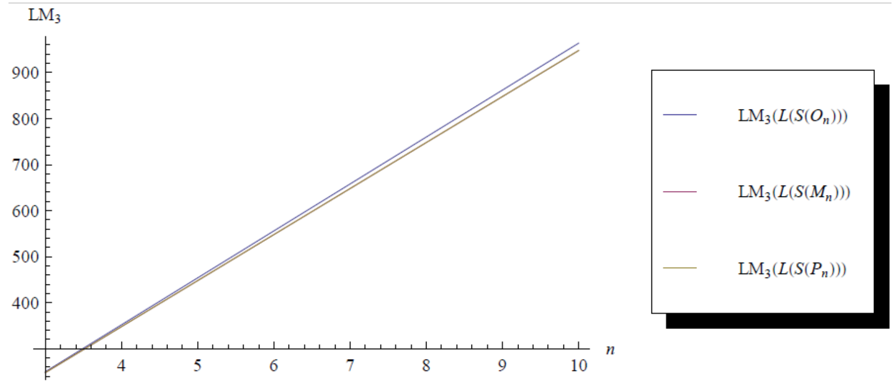

FIGURE 6 Comparison of third leap Zagreb index of the derived graphs of $S(O_n)$, $S(M_n)$ and $S(P_n)$

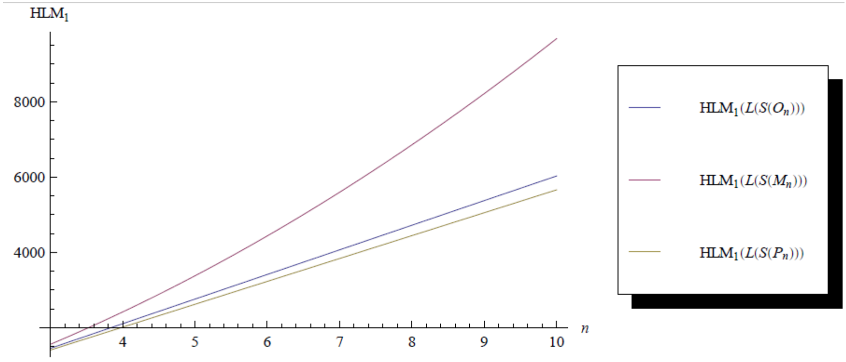

FIGURE 7 Comparison of first leap hyper-Zagreb index of the derived graphs of $S(O_n)$, $S(M_n)$ and $S(P_n)$

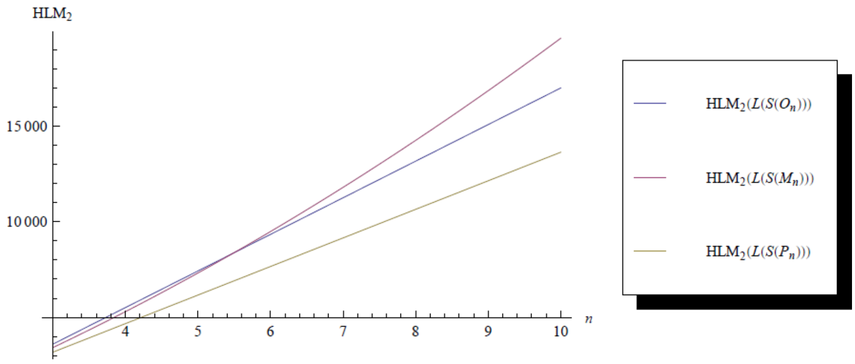

FIGURE 8 Comparison of second leap hyper-Zagreb index of the derived graphs of $S(O_n)$, $S(M_n)$ and $S(P_n)$

Conclusion

The first leap Zagreb index has very good correlation with physical properties of chemical compounds like boiling point, entropy, DHVAP, HVAP and accentric factor. Relying on what stated above, we can conclude that leap indices for ortho-phenyl chain has shown good and quick response whereas leap indices for meta and para-polyphenyl chains mostly behaved alike. We have computed and compared leap Zagreb indices and leap hyper-Zagreb indices of the de-rived graph of the subdivision of certain polyphenyls. These indices can also be computed for further molecular structures.

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