Computation of Leap Adriatic Indices and their Polynomials of Polycyclic Aromatic Hydrocarbons

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Abstract: Adriatic indices are analyzed on the testing sets provided by the International Academy of Mathematical Chemistry (IAMC), these indices were selected as significant predictors of physicochemical properties. In this study, we introduce the certain discrete Adriatic leap indices and their corresponding polynomials of a molecular graph and compute exact formulas for polycyclic aromatic hydrocarbons.

Keywords: Adriatic indices, Adriatic leap indices, polycyclic aromatic hydrocarbon.

Mathematics Subject Classification: 05C05, 05C12, 05C35.

I. Introduction

In Chemical Graph Theory, concerning the definition of the topological index on the molecular graph and concerning chemical properties of drugs can be studied by the topological index calculation see [1]. Numerous degree based topological indices have been appeared in the literature [2] and have found some applications in QSPR/GSAR research [3, 4]. Some of the most useful topological descriptors are bond additive. Adriatic indices were introduced by Vukičević et al. [5] as a way of generalizing well known bond additive indices. Recently some discrete Adriatic indices were studied, for example in [6, 7, 8, 9, 10, 11, 12, 13, 14].

Let $G$ be a finite simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. Let $d_G(u)$ be the number of vertices adjacent to a vertex $u$. The distance $d(u, v)$ between any two vertices $u$ and $v$ of $G$ is the number of edges in a shortest path connecting the vertices $u$ and $v$. For a positive integer $k$, and a vertex $v$ in $G$ is the open neighborhood of $v$ in $G$ is defined as $N_G(v) = \{ u \cup V(G) : d_G(u, v) = k \}$. The $k$-distance degree of a vertex $v$ in $G$ is the number of $k$ neighbors of $v$ in $G$ and it is denoted by $d_k(v)$, see [15]. For undefined term and rotation, we refer [16].

Among those Adriatic indices, the following are some bond additive discrete Adriatic indices [5]:

1. The misbalance indeg index of a graph $G$ is defined as
   \[
   \alpha_1(G) = \sum_{uv \in E(G)} \left| \frac{1}{d_G(u)} - \frac{1}{d_G(v)} \right|
   \]

2. The misbalance hadeg index of a graph $G$ is defined as
   \[
   ha\alpha(G) = \sum_{uv \in E(G)} \left| 2^{-d_G(u)} - 2^{-d_G(v)} \right|
   \]

3. The inverse sum indeg index of a graph $G$ is defined as
   \[
   ISI(G) = \sum_{uv \in E(G)} \frac{d_G(u) d_G(v)}{d_G(u) + d_G(v)}
   \]

4. The symmetric division deg index of $G$ is defined as
   \[
   SD(G) = \sum_{uv \in E(G)} \left( \frac{d_G(u)}{d_G(v)} + \frac{d_G(v)}{d_G(u)} \right)
   \]

Motivated by the Adriatic indices and their wide applications, we introduce the following discrete Adriatic leap indices:

1. The misbalance indeg leap index of $G$ defined as
   \[
   \alpha L_1(G) = \sum_{uv \in E(G)} \left| \frac{1}{d_2(u)} - \frac{1}{d_2(v)} \right|
   \]

2. The misbalance indeg leap index of $G$ is defined as
   \[
   \alpha L_1(G) = \sum_{uv \in E(G)} \left| \frac{1}{\sqrt{d_2(u)}} - \frac{1}{\sqrt{d_2(v)}} \right|
   \]
The misbalance rodeg leap index of $G$ is defined as
$$\alpha L_1(G) = \sum_{uv \in E(G)} \left| \frac{1}{d_1^2(u)} - \frac{1}{d_1^2(v)} \right|.$$  

The misbalance deg leap index (or minus leap index [17]) of $G$ defined as
$$\alpha L_1(G) = \sum_{uv \in E(G)} \frac{d_2(u) - d_2(v)}{d_2(u) + d_2(v)}.$$  

The misbalance sdeg leap index of $G$ is defined as
$$\alpha L_2(G) = \sum_{uv \in E(G)} \left| d_2(u) - d_2(v) \right|.$$  

The general misbalance deg leap index of $G$ is defined as
$$\alpha L_a(G) = \sum_{uv \in E(G)} \left| x^{d_1(u) - d_1(v)} - x^{d_2(u) - d_2(v)} \right|.$$  

The inverse sum indeg leap index of $G$ was defined by Kulli in [18] as
$$ISL(G) = \sum_{uv \in E(G)} \frac{d_2(u) - d_2(v)}{d_2(u) + d_2(v)}.$$  

The symmetric division deg leap index of $G$ is defined as
$$SDL(G) = \sum_{uv \in E(G)} \left( \frac{d_2(u)}{d_2(u) + d_2(v)} \right).$$

Considering bond additive discrete Adriatic leap indices, we introduce the discrete Adriatic leap polynomials as follows:

The misbalance indeg leap polynomial of $G$ is defined as
$$\alpha L_1(G, x) = \sum_{uv \in E(G)} \frac{1}{d_1^2(u)} \cdot \frac{1}{d_1^2(v)}.$$  

The misbalance ideg leap polynomial of $G$ is defined as
$$\alpha L_1(G, x) = \sum_{uv \in E(G)} \frac{1}{d_1^2(u)} \cdot \frac{1}{d_1^2(v)}.$$  

The misbalance rodeg leap polynomial of $G$ is defined as
$$\alpha L_2(G, x) = \sum_{uv \in E(G)} \frac{d_2(u) - d_2(v)}{d_2(u) + d_2(v)}.$$  

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The general misbalance deg leap polynomial of $G$ is defined as
$$\alpha L_a(G, x) = \sum_{uv \in E(G)} \left| x^{d_1(u) - d_1(v)} - x^{d_2(u) - d_2(v)} \right|.$$  

where $a$ is a real number.

The misbalance hadeg leap polynomial of $G$ is defined as
$$h\alpha L(G, x) = \sum_{uv \in E(G)} \left[ 2^{-d_1(u)} - 2^{-d_1(v)} \right].$$

The inverse sum indeg leap polynomial of $G$ is defined as
$$ISL(G, x) = \sum_{uv \in E(G)} \frac{d_2(u) - d_2(v)}{d_2(u) + d_2(v)}.$$
The symmetric division deg leap polynomial of $G$ is defined as

$$ISL(G,x) = \sum_{uv \in E(G)} x^{d_2(u) - d_2(v)}.$$

The symmetric division deg leap polynomial of $G$ is defined as

$$SDL(G,x) = \sum_{uv \in E(G)} x^{d_2(u) - d_2(v)}.$$

Recently some polynomials were studied, for example, in [19, 20].

In this paper, we establish some results on the discrete Adriatic leap indices and their corresponding polynomials for polycyclic aromatic hydrocarbons.

### II. Results for Polycyclic Aromatic Hydrocarbons

We consider the family of polycyclic aromatic hydrocarbons, which is denoted by $PAH_{n}$. We give the first three members of the family $PAH_{n}$ in Figure 1.

![Figure 1. The first three members of $PAH_{n}$](image)

Let $G$ be the molecular graph of $PAH_{n}$. By calculation, $G$ has $6n^2 + 6n$ vertices and $9n^2 + 3n$ edges. For an edge $uv \in E(G)$, the 2-distance degree of a vertex $u$ and a vertex $v$ are respectively denoted by $d_2(u)$ and $d_2(v)$. By calculation we obtain that the edge partition of $G$ with respect to 2-distance degree of vertices is given in Table 1.

<table>
<thead>
<tr>
<th>$d_2(u)$, $d_2(v)$ \ $uv \in E(G)$</th>
<th>(2, 4)</th>
<th>(4, 4)</th>
<th>(4, 6)</th>
<th>(6, 6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of edges</td>
<td>6n</td>
<td>6</td>
<td>$2n^2 + 2n$</td>
<td>$7n^2 - 48n - 6$</td>
</tr>
</tbody>
</table>

**Table 1. Edge partition of $G$ based on $d_2(u)$ and $d_2(v)$**

**Theorem 1.** The general misbalance deg leap index of $PAH_{n}$ is

$$\alpha L_n(PAH_n) = |2^a - 4^a|6n + |4^a - 6^a|(2n^2 + 2n).$$

**Proof:** By using definition and Table 1 we deduce

$$\alpha L_n(PAH_n) = \sum_{uv \in E(G)} |d_2(u)^a - d_2(v)^a|$$

$$= |2^a - 4^a|6n + |4^a - 6^a|6 + |4^a - 6^a|(2n^2 + 2n) + |6^a - 6^b|(7n^2 - 5n - 6)$$

$$= |2^a - 4^a|6n + |4^a - 6^a|(2n^2 + 2n).$$

Using Theorem 1, we obtain the following results.

**Corollary 1.1.** Let $PAH_{n}$ be the family of polycyclic aromatic hydrocarbons. Then

(i) $\alpha L_{2,1}(PAH_n) = \frac{1}{6}n^2 + \frac{4}{3}n.$

(ii) $\alpha L_{1,2}(PAH_n) = \frac{\sqrt{6} - 2}{\sqrt{6}} \times n^2 + \left(\frac{6}{\sqrt{2}} - \frac{2}{\sqrt{6}} - 2\right)n.$

(iii) $\alpha L_{3,1}(PAH_n) = (\sqrt{6} - 2)2n^2 + (8 - 6\sqrt{2} - 2\sqrt{6})n.$

(iv) $\alpha L_{1,3}(PAH_n) = 4n^2 + 16n.$

(v) $\alpha L_{2,3}(PAH_n) = \frac{5}{72}n^2 + \frac{43}{36}n.$
Theorem 2. The general misbalance deg leap Polynomial of PAH is
\[ \alpha L_n(PAH_n, x) = 6nx^{2n-4} + (2n^2 + 2n)x^{4n-6} + (7n^2 - 5n)x^0. \]

Proof: Using definition and Table 1, we derive
\[ \alpha L_n(PAH_n, x) = \sum_{u \in E(G)} x^{d_u(a) - d_v(a)} \]
\[ = 6nx^{2n-4} + 6x^{4n-6} + (2n^2 + 2n)x^{4n-6} + (7n^2 - 5n)x^6. \]
After simplification, we get the desired result.

From Theorem 2, we establish the following results.

Corollary 2.2. Let PAH be the family of polycyclic aromatic hydrocarbons. Then

(i) \[ \alpha L_1(PAH_n, x) = 6nx + (2n^2 + 2n)x^{12} + (7n^2 - 5n)x^0. \]

(ii) \[ \alpha L_2(PAH_n, x) = 6nx^{2n-4} + (2n^2 + 2n)x^{4n-6} + (7n^2 - 5n)x^6. \]

(iii) \[ \alpha L_3(PAH_n, x) = (2n^2 + 8n)x^2 + (7n^2 - 5n)x^5. \]

(iv) \[ \alpha L_4(PAH_n, x) = 3n^{16} + (2n^2 + 2n)x^{144} + (7n^2 - 5n)x^3. \]

(v) \[ \alpha L_5(PAH_n, x) = 6nx^{2n-4} + 6x^{4n-6} + (2n^2 + 2n)x^{4n-6} + (7n^2 - 5n)x^6. \]

Theorem 3. Let PAH be the family of polycyclic aromatic hydrocarbons. Then

(i) \[ h \alpha L_n(PAH_n, x) = \frac{3}{32}x^{n^2} + \frac{39}{32}x^n. \]

(ii) \[ h \alpha L_n(PAH_n, x) = \frac{3}{32}x^{n^2} + \frac{39}{32}x^n. \]

Proof: By using definitions and Table 1, we obtain

(i) \[ h \alpha L_n(PAH_n, x) = \sum_{u \in E(G)} |2^{d_u(a) - d_v(a)}| \]
\[ = 2^{-2} - 2^{-4} |6n + 2^{2n-4} - 2^{-4}| + 2^{-6} - 2^{-6} |7n^2 - 5n - 6| \]
\[ = \frac{3}{32}x^{n^2} + \frac{39}{32}x^n. \]

(ii) \[ h \alpha L_n(PAH_n, x) = \sum_{u \in E(G)} x^{d_u(a) - d_v(a)} \]
\[ = 6nx^{2n-2} + 6x^{4n-6} + (2n^2 + 2n)x^{4n-6} + (2n^2 - 5n - 6)x^6. \]
We obtain the desired result after simplification.

Theorem 4. Let PAH be the family of polycyclic aromatic hydrocarbons. Then

(i) \[ ISL_n(PAH_n) = \frac{24}{5}x^{n^2} - \frac{11}{5}x^n - 6. \]

(ii) \[ ISL_n(PAH_n, x) = 6nx^3 + 6x^2 + (2n^2 + 2n)x^3 + (7n^2 - 5n - 6)x^3. \]

Proof: By using definitions and Table 1, we have
(i) \[ ISL(PAH_n) = \sum_{uv \in E(G)} d_u^2(u)d_v^2(v) \]
\[= \left(\frac{2 \times 4}{2 + 4}\right)6n + \left(\frac{4 \times 4}{4 + 4}\right)6 + \left(\frac{4 \times 6}{4 + 6}\right)(2n^2 + 2n) + \left(\frac{6 \times 6}{6 + 6}\right)(7n^2 - 5n - 6). \]

After simplification, we get the desired result.

(ii) \[ ISL(PAH_n, x) = \sum_{uv \in E(G)} \frac{d_u^3(u)d_v^3(v)}{x^{d_u^2(u)+d_v^2(v)}} \]
\[= 6nx^{2+4} + 6x^{3+4} + (2n^2 + 2n)x^{4+6} + (7n^2 - 5n - 6)x^{6+6}. \]

After simplification, we get the desired result.

**Theorem 5.** Let \( PAH_n \) be the family of polycyclic aromatic hydrocarbons. Then

(i) \[ SDL(PAH_n) = \frac{55}{3} \times n^2 + \frac{28}{3} \times n. \]

(ii) \[ SDL(PAH_n, x) = 6nx^{2+4} + (2n^2 + 2n)x^{5+6} + (7n^2 - 5n - 6)x^6. \]

**Proof:** Using definitions and Table 1, we deduce

(i) \[ SDL(PAH_n) = \sum_{uv \in E(G)} \frac{d_u^3(u)d_v^3(v)}{d_u^2(u)+d_v^2(v)} \]
\[= \left(\frac{2}{4}\right)6n + \left(\frac{4}{4}\right)6 + \left(\frac{4}{6}\right)(2n^2 + 2n) + \left(\frac{6}{6}\right)(7n^2 - 5n - 6)\]
\[= \frac{55}{3} \times n^2 + \frac{28}{3} \times n. \]

(ii) \[ SDL(PAH_n, x) = \sum_{uv \in E(G)} \frac{d_u^3(u)d_v^3(v)}{x^{d_u^2(u)+d_v^2(v)}} \]
\[= 6nx^{2+4} + 6x^{3+4} + (2n^2 + 2n)x^{4+6} + (7n^2 - 5n - 6)x^6. \]

After simplification, we get the desired result.

**Conclusion**

In this study, we have introduced the certain discrete Adriatic leap indices and their corresponding polynomials of a molecular graph. Furthermore, we have computed these newly defined discrete Adriatic leap indices and their corresponding polynomials for very useful nanostructure polycyclic aromatic hydrocarbons. It would also be interesting to compute these adriatic leap indices and their Polynomials for other nanostructures.

**REFERENCES**


