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 $N_k(v/G) = \{u \square V(G) : d(u, v) = k\}$. 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]:
The misbalance indeg index of a graph G is defined as

$$\alpha_{-1}(G) = \sum_{uv \in E(G)} \left| \frac{1}{d_G(u)} - \frac{1}{d_G(v)} \right|.$$

The misbalance hadeg index of a graph G is defined as

$$h\alpha(G) = \sum_{uv \in E(G)} \left| 2^{-d_G(u)} - 2^{-d_G(v)} \right|.$$

The inverse sum indeg index of a graph G is defined as

$$ISI(G) = \sum_{uv \in E(G)} \frac{d_G(u)d_G(v)}{d_G(u) + d_G(v)}.$$

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:
The misbalance indeg leap index of G defined as

$$\alpha L_{-1}(G) = \sum_{uv \in E(G)} \left| \frac{1}{d_2(u)} - \frac{1}{d_2(v)} \right|.$$

The misbalance irdeg leap index of G is defined as

$$\alpha L_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \left| \frac{1}{\sqrt{d_2(u)}} - \frac{1}{\sqrt{d_2(v)}} \right|.$$

The misbalance rodeg leap index of G is defined as

$$\alpha L_{\frac{1}{2}}(G) = \sum_{uv \in E(G)} \left| \sqrt{d_2(u)} - \sqrt{d_2(v)} \right|.$$

The misbalance deg leap index (or minus leap index [17]) of G defined as

$$\alpha L_1(G) = \sum_{uv \in E(G)} \left| d_2(u) - d_2(v) \right|.$$

The misbalance sdeg leap index of G is defined as

$$\alpha L_{-2}(G) = \sum_{uv \in E(G)} \left| \frac{1}{d_2(u)^2} - \frac{1}{d_2(v)^2} \right|.$$

The general misbalance deg leap index of G is defined as

$$\alpha L_a(G) = \sum_{uv \in E(G)} \left| d_2(u)^a - d_2(v)^a \right|.$$

The misbalance hadeg leap index of G is defined as

$$h\alpha L(G) = \sum_{uv \in E(G)} \left| 2^{-d_2(u)} - 2^{-d_2(v)} \right|.$$

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

$$SDL(G) = \sum_{uv \in E(G)} \left(\frac{d_2(u)}{d_2(v)} + \frac{d_2(v)}{d_2(u)} \right).$$

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

$$\alpha L_{-1}(G, x) = \sum_{uv \in E(G)} x^{\left| \frac{1}{d_2(u)} - \frac{1}{d_2(v)} \right|}.$$

The misbalance irdeg leap polynomial of G is defined as

$$\alpha L_{-\frac{1}{2}}(G, x) = \sum_{uv \in E(G)} x^{\left| \frac{1}{\sqrt{d_2(u)}} - \frac{1}{\sqrt{d_2(v)}} \right|}.$$

The misbalance rodeg leap polynomial of G is defined as

$$\alpha L_{\frac{1}{2}}(G, x) = \sum_{uv \in E(G)} x^{\left| \sqrt{d_2(u)} - \sqrt{d_2(v)} \right|}.$$

The misbalance deg leap polynomial of G is defined as

$$\alpha L_1(G, x) = \sum_{uv \in E(G)} x^{\left| d_2(u) - d_2(v) \right|}.$$

The misbalance sdeg leap polynomial of G is defined as

$$\alpha L_{-2}(G, x) = \sum_{uv \in E(G)} x^{\left| \frac{1}{d_2(u)^2} - \frac{1}{d_2(v)^2} \right|}.$$

The general misbalance deg leap polynomial of G is defined as

$$\alpha L_a(G, x) = \sum_{uv \in E(G)} x^{\left| d_2(u)^a - d_2(v)^a \right|}.$$

where a is a real number.

The misbalance hadeg leap polynomial of G is defined as

$$h\alpha L(G, x) = \sum_{uv \in E(G)} x^{\left| 2^{-d_2(u)} - 2^{-d_2(v)} \right|}.$$

The inverse sum indeg leap polynomial of G is defined as

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

The symmetric division deg leap polynomial of G is defined as

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

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.
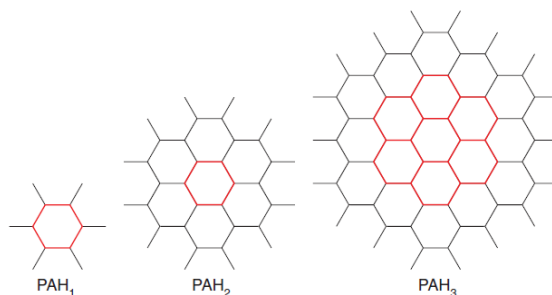

Figure 1. The first three members of PAH_n

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 $uv \square E(G)$, 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.

$d_2(u), d_2(v) \backslash uv \square E(G)$	(2, 4)	(4, 4)	(4, 6)	(6, 6)
Number of edges	$6n$	6	$2n^2 + 2n$	$7n^2 - 48n - 6$

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

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

Proof: By using definition and Table 1 we deduce

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

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

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

Using Theorem 1, we obtain the following results.

Corollary 1.1. Let PAH_n be the family of polycyclic aromatic hydrocarbons. Then

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

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

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

(iv) $\alpha L_1(PAH_n) = 4n^2 + 16n.$

(v) $\alpha L_{-2}(PAH_n) = \dfrac{5}{72}n^2 + \dfrac{43}{36}n.$

Theorem 2. The general misbalance deg leap Polynomial of PAH_n is

$$\alpha L_a\left(PAH_n, x\right) = 6nx^{|2^a - 4^a|} + \left(2n^2 + 2n\right)x^{|4^a - 6^a|} + \left(7n^2 - 5n\right)x^0.$$

Proof: Using definition and Table 1, we derive

$$\alpha L_a\left(PAH_n, x\right) = \sum_{uv \in E(G)} x^{|d_2(u)^a - d_2(v)^a|}$$

$$= 6nx^{|2^a - 4^a|} + 6x^{|4^a - 4^a|} + \left(2n^2 + 2n\right)x^{|4^a - 6^a|} + \left(7n^2 - 5n - 6\right)x^{|6^a - 6^a|}.$$

After simplification, we get the desired result.

From Theorem 2, we establish the following results.

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

(i) $\quad \alpha L_{-1}\left(PAH_n, x\right) = 6nx^{\frac{1}{4}} + \left(2n^2 + 2n\right)x^{\frac{1}{12}} + \left(7n^2 - 5n\right)x^0.$

(ii) $\quad \alpha L_{-\frac{1}{2}}\left(PAH_n, x\right) = 6nx^{\frac{1}{\sqrt{2}} - \frac{1}{2}} + \left(2n^2 + 2n\right)x^{\frac{1}{2} - \frac{1}{\sqrt{6}}} + \left(7n^2 - 5n\right)x^0.$

(iii) $\quad \alpha L_{\frac{1}{2}}\left(PAH_n, x\right) = 6nx^{2 - \sqrt{2}} + \left(2n^2 + 2n\right)x^{\sqrt{6} - 2} + \left(7n^2 - 5n\right)x^0.$

(iv) $\quad \alpha L_1\left(PAH_n, x\right) = \left(2n^2 + 8n\right)x^2 + \left(7n^2 - 5n\right)x^0.$

(v) $\quad \alpha L_{-2}\left(PAH_n, x\right) = 6nx^{\frac{3}{16}} + \left(2n^2 + 2n\right)x^{\frac{5}{144}} + \left(7n^2 - 5n\right)x^0.$

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

(i) $\quad h\alpha L\left(PAH_n\right) = \frac{3}{32} \times n^2 + \frac{39}{32} \times n.$

(ii) $\quad h\alpha L\left(PAH_n, x\right) = 6nx^{\frac{3}{16}} + \left(2n^2 + 2n\right)x^{\frac{3}{64}} + \left(7n^2 - 5n\right)x^0.$

Proof: By using definitions and Table 1, we obtain

(i) $\quad h\alpha L\left(PAH_n\right) = \sum_{uv \in E(G)} \left|2^{-d_2(u)} - 2^{-d_2(v)}\right|$

$$= \left|2^{-2} - 2^{-4}\right|6n + \left|2^{-4} - 2^{-4}\right|6 + \left|2^{-4} - 2^{-6}\right|\left(2n^2 + 2n\right)$$

$$+ \left|2^{-6} - 2^{-6}\right|\left(7n^2 - 5n - 6\right)$$

$$= \frac{3}{32} \times n^2 + \frac{39}{32}n.$$

(ii) $\quad h\alpha L\left(PAH_n, x\right) = \sum_{uv \in E(G)} x^{|2^{-d_2(u)} - 2^{-d_2(v)}|}$

$$= 6nx^{|2^{-2} - 2^{-4}|} + 6x^{|2^{-4} - 2^{-4}|} + \left(2n^2 + 2n\right)x^{|2^{-4} - 2^{-6}|} + \left(2n^2 - 5n - 6\right)x^{|2^{-6} - 2^{-6}|}.$$

We obtain the desired result after simplification.

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

(i) $\quad ISL\left(PAH_n\right) = \frac{24}{5}n^2 - \frac{11}{5}n - 6.$

(ii) $\quad ISL\left(PAH_n, x\right) = 6nx^{\frac{4}{3}} + 6x^2 + \left(2n^2 + 2n\right)x^{\frac{12}{5}} + \left(7n^2 - 5n - 6\right)x^3.$

Proof: By using definitions and Table 1, we have

(i) $\quad ISL\left(PAH_n\right) = \sum_{uv \in E(G)} \dfrac{d_2(u)d_2(v)}{d_2(u)+d_2(v)}$

$$= \left(\frac{2 \times 4}{2+4}\right)6n + \left(\frac{4 \times 4}{4+4}\right)6 + \left(\frac{4 \times 6}{4+6}\right)\left(2n^2 + 2n\right) + \left(\frac{6 \times 6}{6+6}\right)\left(7n^2 - 5n - 6\right).$$

After simplification, we get the desired result.

(ii) $\quad ISL\left(PAH_n, x\right) = \sum_{uv \in E(G)} x^{\frac{d_2(u)d_2(v)}{d_2(u)+d_2(v)}}$

$$= 6nx^{\frac{2 \times 4}{2+4}} + 6x^{\frac{4 \times 4}{4+4}} + \left(2n^2 + 2n\right)x^{\frac{4 \times 6}{4+6}} + \left(7n^2 - 5n - 6\right)x^{\frac{6 \times 6}{6+6}}.$$

After simplification, we get the desired result.

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

(i) $\quad SDL\left(PAH_n\right) = \dfrac{55}{3} \times n^2 + \dfrac{28}{3} \times n.$

(ii) $\quad SDL\left(PAH_n, x\right) = 6nx^{\frac{5}{2}} + \left(2n^2 + 2n\right)x^{\frac{13}{6}} + \left(7n^2 - 5n\right)x^2.$

Proof: Using definitions and Table 1, we deduce

(i) $\quad SDL\left(PAH_n\right) = \sum_{uv \in E(G)} \left(\dfrac{d_2(u)}{d_2(v)} + \dfrac{d_2(v)}{d_2(u)}\right)$

$$= \left(\frac{2}{4} + \frac{4}{2}\right)6n + \left(\frac{4}{4} + \frac{4}{4}\right)6 + \left(\frac{4}{6} + \frac{6}{4}\right)\left(2n^2 + 2n\right) + \left(\frac{6}{6} + \frac{6}{6}\right)\left(7n^2 - 5n - 6\right)$$

$$= \frac{55}{3} \times n^2 + \frac{28}{3}n.$$

(ii) $\quad SDL\left(PAH_n, x\right) = \sum_{uv \in E(G)} x^{\frac{d_2(u)}{d_2(v)} + \frac{d_2(v)}{d_2(u)}}$

$$= 6nx^{\frac{2}{4}+\frac{4}{2}} + 6x^{\frac{4}{4}+\frac{4}{4}} + \left(2n^2 + 2n\right)x^{\frac{4}{6}+\frac{6}{4}} + \left(7n^2 - 5n - 6\right)x^{\frac{6}{6}+\frac{1}{6}}.$$

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.

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