The (*a, b*)-*KA* Indices of Polycyclic Aromatic Hydrocarbons and Benzenoid Systems

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Abstract: *A chemical graph is a graph such that vertices correspond to the atoms and the edges to the bonds. The graph indices are applied to measure the chemical characteristics of compounds in Chemical Graph Theory. In this paper, we introduce the first and second (a, b)-KA indices of a chemical graph. Furthermore, we study the mathematical properties of these indices for polycyclic aromatic hydrocarbons and benzenoid systems.*

Keywords: *Chemical graph, first (a, b)-KA index, second (a, b)-KA index, polycyclic aromatic hydrocarbon, benzenoid system.*

Mathematics Subject Classification: $05C05$, $05C07$, $05C90$

1. Introduction

A graph index is the numeric quantity from the structural graph of a molecule. Graph indices have been found to be useful in chemical documentation, isomer discrimination, structure property relationships, structure activity relationships and pharmaceutical drug design in Chemistry. There has been considerable interest in the general problem of determining graph indices [1, 2, 3].

Throughout this paper, we consider only finite, simple, connected graphs. Let G be a finite, simple, connected graph. We denote the set of vertices of G by $V(G)$ and the set of edges by $E(G)$. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u. For terms and concepts not given here, we refer [4].

The first and second Zagreb indices [5] of a graph G are defined as

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2 = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v) \right],$$
$$M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

Many properties and chemical applications of these indices can be found in [7,8,9]. Recently, some graph indices were studied in [10,11,12].

In [13], Shirdel et al. proposed the first hyper Zagreb index, defined as

$$HM_1(G) = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v) \right]^2.$$

Some properties of this index were obtained in [14, 15].

The second hyper Zagreb index was defined as [16]

$$HM_2(G) = \sum_{uv \in E(G)} \left[d_G(u) d_G(v) \right]^2.$$

Recently, some new hyper graph indices were studied in [17,18,19,20].

In [21] and [22], the generalization of Zagreb indices were proposed, defined as

$$M_1^{*a}(G) = \sum_{u \in V(G)} d_G(u)^a = \sum_{uv \in E(G)} \left[d_G(u)^{a-1} + d_G(v)^{a-1} \right],$$
$$M_2^a(G) = \sum_{uv \in E(G)} \left[d_G(u) d_G(v) \right]^a,$$

where a is a real number.

In [23], Zhou et al. introduced the general sum connectivity index, defined as

$$M_1^a(G) = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v) \right]^a.$$

The forgotten topological index or F-index is defined as [24]

$$F(G) = \sum_{u \in V(G)} d_G(u)^3 = \sum_{uv \in E(G)} \left[d_G(u)^2 + d_G(v)^2 \right].$$

Many results on $F(G)$ can be found in [25, 26].

In [27], the sum connectivity index was introduced, defined as

$$S(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) + d_G(v)}}.$$

The product connectivity index was introduced by Randić in [28], defined as

$$P(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}.$$

The reciprocal product connectivity index was defined in [29] as

$$RP(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)d_G(v)}.$$

Recently, some new connectivity indices were studied in [30,31,32].

We introduce the first and second (a, b)-KA indices and coindices of a graph G and they are defined as

$$KA^1_{a,b}(G) = \sum_{uv \in E(G)} \left[d_G(u)^a + d_G(v)^a \right]^b,$$

$$\overline{KA}^1_{a,b}(G) = \sum_{uv \notin E(G)} \left[d_G(u)^a + d_G(v)^a \right]^b,$$

$$KA^2_{a,b}(G) = \sum_{uv \in E(G)} \left[d_G(u)^a \, d_G(v)^a \right]^b,$$

$$\overline{KA}^2_{a,b}(G) = \sum_{uv \notin E(G)} \left[d_G(u)^a \, d_G(v)^a \right]^b,$$

where a, b are real numbers.

We easily see that

    (1) $M_1(G) = KA^1_{1,1}(G).$ (2) $HM_1(G) = KA^1_{1,2}(G).$

    (3) $M_1^{*a}(G) = KA^1_{a-1,1}(G).$ (4) $M_1^a(G) = KA^1_{1,a}(G).$

    (5) $F(G) = KA^1_{2,1}(G).$ (6) $S(G) = KA^1_{1,-\frac{1}{2}}(G).$

Furthermore, we also see that

    (1) $M_2(G) = KA^2_{1,1}(G).$ (2) $HM_2(G) = KA^2_{1,2}(G).$

    (3) $M_2^a(G) = KA^2_{1,a}(G) = KA^2_{a,1}(G).$ (4) $P(G) = KA^2_{1,-\frac{1}{2}}(G) = KA^2_{-\frac{1}{2},1}(G).$

    (5) $RP(G) = KA^2_{1,\frac{1}{2}}(G) = KA^2_{\frac{1}{2},1}(G).$

Clearly, we obtain some other graph indices directly as a special case of (a, b)-KA indices for some special values of a and b.

In this paper, we compute the first and second (a, b)-KA indices of polycyclic aromatic hydrocarbons and benzenoid systems.

II. Results for Polycyclic Aromatic Hydrocarbons

We focus on the chemical graph structure of the family polycyclic aromatic hydrocarbons, denoted by PAH_n. The first three members of the family PAH_n are presented in Figure 1.
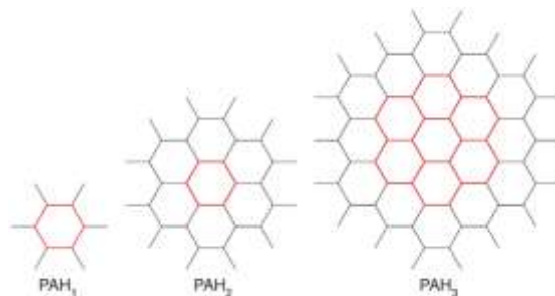
Figure 1

In the following theorem, we determine the first (a, b)-KA index of PAH_n.

Theorem 1. The first (a, b)-KA index of PAH_n is given by

$$KA^1_{a,b}\left(PAH_n\right) = \left(1^a + 3^a\right)^b 6n + \left(2 \times 3^a\right)^b \left(9n^2 - 3n\right). \tag{i}$$

Proof: Let $G = PAH_n$. Clearly, the vertices of G are either of degree 1 or 3, see Figure 1. By calculation, we see that G has $6n^2 + 6n$ vertices and $9n^2 + 3n$ edges. In G, there are two types of edges based on the degree of end vertices of each edge as given in Table 1.

$d_G(u), d_G(v)\backslash uv \in E(G)$	$(1, 3)$	$(3, 3)$
Number of edges	$6n$	$9n^2 - 3n$

Table 1. Edge partition of PAH_n

To compute $KA^1_{a,b}\left(PAH_n\right)$, we see that

$$
\begin{aligned}
KA^1_{a,b}\left(PAH_n\right) &= \sum_{uv \in E(G)} \left[d_G(u)^a + d_G(v)^a\right]^b \\
&= \left(1^a + 3^a\right)^b 6n + \left(3^a + 3^a\right)^b \left(9n^2 - 3n\right) \\
&= \left(1^a + 3^a\right)^b 6n + \left(2 \times 3^a\right)^b \left(9n^2 - 3n\right).
\end{aligned}
$$

We obtain the following results by using equation (i).

Corollary 1.1. Let $G = PAH_n$ be the family of a polycyclic aromatic hydrocarbon. Then

(1) $M_1(G) = KA^1_{1,1}(G) = 54n^2 + 6n.$

(2) $HM_1(G) = KA^1_{1,2}(G) = 324n^2 - 12n.$

(3) $M_1^{*a}(G) = KA^1_{a-1,1}(G) = \left(1^{a-1} + 3^{a-1}\right)6n + \left(2 \times 3^{a-1}\right)\left(9n^2 - 3n\right).$

(4) $M_1^a(G) = KA^1_{1,a}(G) = 9 \times 6^a n^2 + \left(6 \times 4^a - 3 \times 6^a\right)n.$

(5) $F(G) = KA^1_{2,1}(G) = 18n^2 + 6n.$

(6) $S(G) = KA^1_{1,-\frac{1}{2}}(G) = \dfrac{9}{\sqrt{6}}n^2 + \left(1 - \dfrac{1}{\sqrt{6}}\right)3n.$

In the next theorem, we compute the second (a, b)-KA index of PAH_n.

Theorem 2. The second (a, b)-KA index of PAH_n is given by

$$KA^2_{a,b}\left(PAH_n\right) = 9 \times 3^{2ab} n^2 + \left(6 \times 3^{ab} - 3 \times 3^{2ab}\right)n. \tag{ii}$$

Proof: Let $G = PAH_n$. By cardinalities of the edge partition of PAH_n, we have

$$KA^2_{a,b}\left(PAH_n\right) = \sum_{uv \in E(G)} \left[d_G(u)^a \, d_G(v)^a\right]^b$$

$$=\left(1^a \times 3^a\right)^b 6n + \left(3^a \times 3^a\right)^b \left(9n^2 - 3n\right)$$

$$= 9 \times 3^{2ab} n^2 + \left(6 \times 3^{ab} - 3 \times 3^{2ab}\right)n.$$

We establish the following results by equation (ii).

Corollary 2.1. Let $G = PAH_n$ be the family of a polycyclic aromatic hydrocarbon. Then

(1) $M_2(G) = KA_{1,1}^2(G) = 81n^2 - 9n.$

(2) $HM_2(G) = KA_{1,2}^2(G) = 729n^2 - 189n.$

(3) $M_2^a(G) = KA_{1,a}^2(G) = 9 \times 3^{2a} n^2 + \left(6 \times 3^a - 3 \times 3^{2a}\right)n.$

(4) $P(G) = KA_{1,-\frac{1}{2}}^2(G) = 3n^2 + \left(\dfrac{6}{\sqrt{3}} - 1\right)n.$

(5) $RP(G) = KA_{1,\frac{1}{2}}^2(G) = 27n^2 + \left(6\sqrt{3} - 9\right)n.$

III. Results for Benzenoid Systems

We focus on the chemical graph structure of a jagged rectangle benzenoid system, denoted by $B_{m,n}$ for all m, n, in N. Three chemical graphs of a jagged rectangle benzenoid system are depicted in Figure 2.
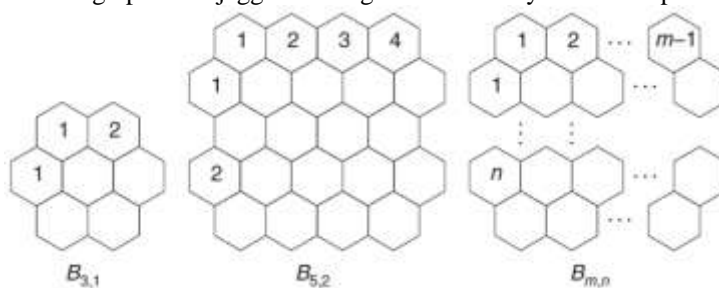

Figure 2

In the following theorem, we determine the first (a, b)-KA index of $B_{m,n}$.

Theorem 3. Let $B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then

$$KA_{a,b}^1\left(B_{m,n}\right) = \left(2^a + 2^a\right)^b (2n+4) + \left(2^a + 3^a\right)^b (4m+4n-4)$$

$$+ \left(3^a + 3^a\right)^b (6mn + m - 5n - 4). \qquad \text{(iii)}$$

Proof: Let $H = B_{m,n}$. Clearly the vertices of H are either of degree 2 or 3, see Figure 2. By calculation, we obtain that H has $4mn + 4m + m - 2$ vertices and $6mn + 5m + n - 4$ edges. In H, there are three types of edges based on the degree of end vertices of each edge as given in Table 2.

$d_H(u)\, d_H(v) \backslash uv \in E(H)$	(2,2)	(2,3))	(3, 3)
Number of edges	$2n+4$	$4m+4n-4$	$6mn + m - 5n - 4$

Table 2. Edge partition of $B_{m,n}$

To compute $KA_{a,b}^1\left(B_{m,n}\right)$, we see that

$$KA_{a,b}^1\left(B_{m,n}\right) = \sum_{uv \in E(H)} \left[d_H(u)^a + d_H(v)^a\right]^b$$

$$= \left(2^a + 2^a\right)^b (2n+4) + \left(2^a + 3^a\right)^b (4m+4n-4) + \left(3^a + 3^a\right)^b (6mn + m - 5n - 4).$$

We establish the following results by using equation (iii).

Corollary 3.1. Let $H = B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then

(1) $M_1(H) = KA^1_{1,1}(H) = 36mn + 26m - 2n - 28.$

(2) $HM_1(H) = KA^1_{1,2}(H) = 216mn + 136m - 48n - 180.$

(3) $M_1^{*a}(H) = KA^1_{a-1,1}(H) = 2 \times 2^{a-1}(2n+4) + \left(2^{a-1} + 3^{a-1}\right)(4m + 4n - 4)$
$$+ 2 \times 3^{a-1}(6mn + m - 5n - 4).$$

(4) $M_1^a(H) = KA^1_{1,a}(H) = 4^a(2n+4) + 5^a(4m + 4n - 4) + 6^a(6mn + m - 5n - 4).$

(5) $F(H) = KA^1_{2,1}(H) = 108mn + 70m - 22n - 92.$

(6) $S(H) = KA^1_{1,-\frac{1}{2}}(H) = \frac{1}{\sqrt{4}}(2n+4) + \frac{1}{\sqrt{5}}(4m + 4n - 4) + \frac{1}{\sqrt{6}}(6mn + m - 5n - 4).$

In the next theorem, we compute the second (a, b)-KA index of $B_{m,n}$.

Theorem 4. Let $B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then
$$KA^2_{a,b}(B_{m,n}) = \left(2^a \times 2^a\right)^b(2n+4) + \left(2^a \times 3^a\right)^b(4m + 4n - 4)$$
$$+ \left(3^a \times 3^a\right)^b(6mn + m - 5n - 4). \qquad (iv)$$

Proof: Let $H = B_{m,n}$. By cardinalities of the edge partition of $B_{m,n}$, we obtain

$$KA^2_{a,b}(B_{m,n}) = \sum_{uv \in E(H)} \left[d_H(u)^a\, d_H(v)^a\right]^b$$
$$= \left(2^a \times 2^a\right)^b(2n+4) + \left(2^a \times 3^a\right)^b(4m + 4n - 4) + \left(3^a \times 3^a\right)^b(6mn + m - 5n - 4).$$

We obtain the following results by using equation (iv).

Corollary 4.1. Let $H = B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then

(1) $M_2(H) = KA^2_{1,1}(H) = 54mn + 33m - 13n - 28.$

(2) $HM_2(H) = KA^2_{1,2}(H) = 486mn + 225m - 229n - 404.$

(3) $M_2^a(H) = KA^2_{1,a}(H) = KA^2_{a,1}(H) = 6 \times 9^a mn + \left(4 \times 6^a + 9^a\right)m$
$$+ \left(2 \times 4^a + 4 \times 6^a - 5 \times 9^a\right)n + \left(4 \times 4^a - 4 \times 6^a - 4 \times 9^a\right)$$

(4) $P(H) = KA^2_{1,-\frac{1}{2}}(H) = KA^2_{-\frac{1}{2},1}(H) = 2mn + \left(\frac{4}{\sqrt{6}} + \frac{1}{3}\right)m + \left(\frac{4}{\sqrt{6}} - \frac{2}{3}\right)n - \left(\frac{4}{\sqrt{6}} + \frac{2}{3}\right).$

(5) $RP(H) = KA^2_{1,\frac{1}{2}}(H) = KA^2_{\frac{1}{2},1}(H) = 18mn + \left(4\sqrt{6} + 3\right)m + \left(4\sqrt{6} - 11\right)n - \left(4\sqrt{6} + 4\right).$

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