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Reduced (*a*, *b*)-*KA* Indices of Benzenoid Systems

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Abstract. Topological indices are applied to measure the chemical characteristics of chemical compounds. This study computes the reduced (*a*, *b*)-*KA* indices of benzenoid systems. Also, we obtain some other reduced graph indices directly as special values of *a* and *b.*

Keywords: reduced (*a*,*b*)-*KA* indices, benzenoid system

AMS Mathematics Subject Classification (2010): 05*C*05, 05*C*07, 05*C*35

1. Introduction

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. We refer [1], for other undefined notations and terminologies.

A molecular graph is a graph such that its vertices correspond to the atoms and edges to the bonds. Chemical Graph Theory is a branch of mathematical chemistry, which has an important effect on the development of Chemical Sciences. Several topological indices have been considered in Theoretical Chemistry and have found some applications.

The reduced first Zagreb index [2] of a graph G is defined as

$$RM_1(G) = \sum_{uv \in E(G)} \left[\left(d_G(u)-1\right) + \left(d_G(v)-1\right) \right] = \sum_{e \in E(G)} d_G(e).$$

In [3], Furtula et al. proposed the reduced second Zagreb index, defined as

$$RM_2(G) = \sum_{uv \in E(G)} \left(d_G(u)-1\right)\left(d_G(v)-1\right).$$

In [4], Milicevic et al. introduced the reduced first hyper Zagreb index(or reformulated first Zagreb index) of a graph G, defined it as

$$RHM_1(G) = \sum_{uv \in E(G)} \left[\left(d_G(u)-1\right) + \left(d_G(v)-1\right) \right]^2 == \sum_{e \in E(G)} d_G(e)^2 = EM_1(G).$$

In [5], Kulli introduced the K-edge index of a graph G, defined as

$$K_e(G) = \sum_{uv \in E(G)} \left[\left(d_G(u)-1\right) + \left(d_G(v)-1\right) \right]^3 = \sum_{e \in E(G)} d_G(e)^3.$$

In [6], Kulli introduced the reduced second hyper-Zagreb index of a graph G, defined as,

$$RHM_2(G)=\sum_{uv\in E(G)}\left[\left(d_G(u)-1\right)\left(d_G(v)-1\right)\right]^2.$$

We now define the reduced modified first Zagreb and reduced sum connectivity indices of a graph G as

$$^{m}RM_1(G)=\sum_{uv\in E(G)}\frac{1}{\left(d_G(u)-1\right)+\left(d_G(v)-1\right)}=\sum_{e\in E(G)}\frac{1}{d_G(e)}.$$

$$RS(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{\left(d_G(u)-1\right)+\left(d_G(v)-1\right)}}=\sum_{e\in E(G)}\frac{1}{\sqrt{d_G(e)}}.$$

The reduced modified first Zagreb and reduced product connectivity indices of a graph G were introduced by Kulli in [7] and they are defined as

$$^{m}RM_2(G)=\sum_{uv\in E(G)}\frac{1}{\left(d_G(u)-1\right)\left(d_G(v)-1\right)}.$$

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

We define the reciprocal reduced product connectivity index of G as

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

In [8], Kulli defined the general reduced Zagreb index of G as

$$RM_1^a(G)=\sum_{uv\in E(G)}\left[\left(d_G(u)-1\right)+\left(d_G(v)-1\right)\right]^a=\sum_{e\in E(G)}\left[d_G(e)\right]^a.$$

The general reduced second Zagreb index was defined by Kulli in [9] as

$$RM_2^a(G)=\sum_{uv\in E(G)}\left[\left(d_G(u)-1\right)\left(d_G(v)-1\right)\right]^a.$$

We now define the reduced F-index of G as

$$RF(G)=\sum_{uv\in E(G)}\left[\left(d_G(u)-1\right)^2+\left(d_G(v)-1\right)^2\right].$$

We now define the general reduced Zagreb index of G as

$$RM^a(G)=\sum_{uv\in E(G)}\left[\left(d_G(u)-1\right)^a+\left(d_G(v)-1\right)^a\right].$$

In [10], Gutman introduced the reduced Sombor index of a graph G, defined as

$$RSO(G)=\sum_{uv\in E(G)}\sqrt{\left(d_G(u)-1\right)^2+\left(d_G(v)-1\right)^2}.$$

Recently, some Sombor indices were studied in [11,12,13,14,15,16,17,18,19,20].

The reduced modified Sombor index was introduced by Kulli et al. in [21] and it is defined as

$$^{m}RSO(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{\left(d_G(u)-1\right)^2+\left(d_G(v)-1\right)^2}}.$$

In [21], Kulli et al. introduced the first and second reduced (*a*, *b*)-*KA* indices of a graph *G*, defined as

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

$$RKA^2_{a,b}(G)=\sum_{uv\in E(G)}\left[\left(d_G(u)-1\right)^a\left(d_G(v)-1\right)^a\right]^b,$$

where *a*, *b* are real numbers.
We easily see that

(1) $RM_1(G)=RKA^1_{1,1}(G)$. (2) $HRM_1(G)=RKA^1_{1,2}(G)$.

(3) $RM_1^a(G)=RKA^1_{1,a}(G)$. (4) $RM^a(G)=RKA^1_{a,1}(G)$.

(5) ${}^mRM_1(G)=RKA^1_{1,-1}(G)$. (6) $RS(G)=RKA^1_{1,-\frac{1}{2}}(G)$.

(7) $K_e(G)=RKA^1_{1,3}(G)$. (8) $RF(G)=RKA^1_{2,1}(G)$.

(9) $RSO(G)=RKA^1_{2,\frac{1}{2}}(G)$. (10) ${}^mRSO(G)=RKA^1_{2,-\frac{1}{2}}(G)$.

Furthermore, we also see that

(1) $RM_2(G)=RKA^2_{1,1}(G)$. (2) $HRM_2(G)=RKA^2_{1,2}(G)$.

(3) $RM_2^a(G)=RKA^2_{1,a}(G)$ (4) ${}^mRM_2(G)=RKA^2_{1,-1}(G)$.

(5) $RP(G)=RKA^2_{1,-\frac{1}{2}}(G)$. (6) $RRP(G)=RKA^2_{1,\frac{1}{2}}(G)$.

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

In this paper, we compute the first and second reduced (*a*, *b*)-*KA* indices for benzenoid systems. For benzenoid systems, see [22].

2. 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 1.

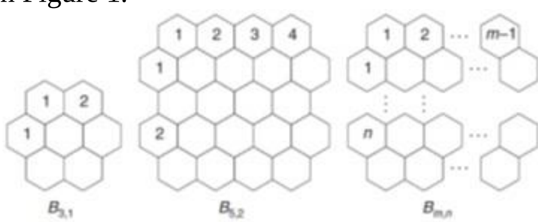

Figure 1: Jagged rectangle benzenoid system

Let $H = B_{m,n}$. Clearly the vertices of *H* are either of degree 2 or 3, see Figure 1. 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 1.

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

Table 1: Edge partition of $B_{m,n}$

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

Theorem 1. Let $B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then

$$KA^1_{a,b}\left(B_{m,n}\right)=2^b\left(2n+4\right)+\left(1^a+2^a\right)^b\left(4m+4n-4\right)$$
$$+\left(2^a+2^a\right)^b\left(6mn+m-5n-4\right).$$

Proof: Let $G = HC_5C_7[p,q]$. By using equation (7) and Table 1, we deduce

$$RKA^1_{a,b}\left(B_{m,n}\right)=\sum_{uv\in E(G)}[(d_G(u)-1)^a+\left(d_{G(v)}-1\right)^a]^b$$
$$=[(2-1)^a+(2-1)^a]^b(2n+4)$$
$$+[(2-1)^a+(3-1)^a]^b(4m+4n-4)$$
$$+[(3-10)^a+(3-1)^a]^b\,(6mn+m-5n-4)$$

After simplification, we get the desired result.

We establish the following results by using Theorem 1.

Corollary 1.1. Let $G = B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then

(1) $RM_1(G)=RKA^1_{1,1}(G)=24mn+16m-4n-20.$

(2) $HRM_1(G)=RKA^1_{1,2}(G)=96mn+52m-36n-84.$

(3) $RM_1^a(G)=RKA^1_{1,a}(G)=6\times 4^a mn+\left(4\times 3^a+4^a\right)m+\left(2\times 2^a+4\times 3^a-5\times 4^a\right)n$
$$+\left(4\times 2^a-4\times 3^a-4\times 4^a\right).$$

(4) $RM^a(G)=RKA^1_{a,1}(G)=12\times 2^a mn+\left(6+5\times 2^a\right)m+\left(8-6\times 2^a\right)n+6^a\left(4-12\times 2^a\right).$

(5) ${}^mRM_1(G)=RKA^1_{1,-1}(G)=\frac{3}{2}mn+\frac{19}{12}70m+\frac{13}{12}n-\frac{1}{3}.$

(6) $RS(G)=RKA^1_{1,-\frac{1}{2}}(G)=3mn+\left(\frac{4}{\sqrt{3}}+\frac{1}{2}\right)m+\left(\frac{2}{\sqrt{2}}+\frac{4}{\sqrt{3}}-\frac{5}{2}\right)n+\left(\frac{4}{\sqrt{2}}-\frac{4}{\sqrt{3}}-2\right)$

(7) $K_e(G)=RKA^1_{1,3}(G)=384mn+172m-196n-332.$

(8) $RF(G)=RKA^1_{2,1}(G)=48mn+28m-16n-44.$

(9) $RSO(G)=RKA^1_{2,\frac{1}{2}}(G)=12\sqrt{2}mn+(4\sqrt{5}+2\sqrt{2})m+\left(4\sqrt{5}-8\sqrt{2}\right)n-(4\sqrt{5}+4\sqrt{2}).$

(10) $\quad {}^{m}RSO(G) = RKA^{1}_{2,-\frac{1}{2}}(G) = \frac{3}{\sqrt{2}}mn + \left(\frac{4}{\sqrt{5}} + \frac{1}{2\sqrt{2}}\right)m + \left(\frac{4}{\sqrt{5}} - \frac{1}{2\sqrt{2}}\right)n + \left(\frac{2}{\sqrt{2}} - \frac{4}{\sqrt{5}}\right)$

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

Theorem 2. Let $B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then

$$RKA^{1}_{a,b}\left(B_{m,n}\right) = (2n+4) + 2^{ab}(4m+4n-4) + 2^{2ab}(6mn+m-5n-4).$$

Proof: Let $G = B_{m,n}$. By definition and Table 1, we deduce

$$\begin{aligned} RKA^{1}_{a,b}\left(B_{m,n}\right) &= \sum_{uv\in E(G)} [(d_G(u)-1)^a + (d_G(v)-1)^a]^b \\ &= [(2-1)^a \times (2-1)^a]^b(2n+4) \\ &\quad +[(2-1)^a \times (3-1)^a]^b(4m+4n-4) \\ &\quad +[(3-10)^a \times (3-1)^a]^b\,(6mn+m-5n-4) \end{aligned}$$

After simplification, we get the desired result.

We establish the following results by using Theorem 2.

Corollary 2.1. Let $G = B_{m,n}$ be the family of a jagged rectangle benzenoid system. Then

(1) $RM_2(G) = RKA^{2}_{1,1}(G) = 24mn + 12m - 10n - 20.$

(2) $HRM_2(G) = RKA^{2}_{1,2}(G) = 96mn + 32m - 62n - 76.$

(3) $RM_2^{a}(G) = RKA^{2}_{1,a}(G)$

$$= 6\times 2^{2a}mn + \left(4\times 2^{a} + 2^{2a}\right)m + \left(2 + 4\times 2^{a} - 5\times 2^{a}\right)n + \left(4 - 4\times 2^{a} - 4\times 2^{2a}\right) \qquad (4)$$

${}^{m}RM_2(G) = RKA^{2}_{1,-1}(G) = \frac{3}{2}mn + \frac{9}{4}m + \frac{11}{4}n + 1.$

(5) $RP(G) = RKA^{2}_{1,-\frac{1}{2}}(G) = 3mn + \left(2\sqrt{2} + \frac{1}{2}\right)m + \left(2\sqrt{2} - \frac{1}{2}\right)n + \left(2 - 2\sqrt{2}\right).$

(6) $RRP(G) = RKA^{2}_{1,\frac{1}{2}}(G) = 12mn + (4\sqrt{2}+2)m + \left(4\sqrt{2} - 8\right)n - (4 + 4\sqrt{2}).$

3. Conclusion

In this paper, we have introduced the reduced modified first Zagreb index, reduced sum connectivity index, reciprocal reduced product connectivity index, reduced *F*-index, general reduced Zagreb index of a graph. We have determined the first and second reduced (*a*, *b*)-*KA* indices of benzenoid systems. Furthermore, for some particular values of *a* and *b*, we have computed some other reduced topological indices directly as a special case of reduced (*a*, *b*)-*KA* indices.

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