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On Reduced Zagreb Indices of Polycyclic Aromatic Hydrocarbons and Benzenoid Systems

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Abstract. In this paper, we introduce the reduced modified first Zagreb index, reduced inverse degree index, reduced zeroth-order Randić index, reduced F-index and generalized reduced first Zagreb index of a graph. Also we determine these indices for polycyclic aromatic hydrocarbons and jagged rectangle benzenoid systems.

Keywords: reduced Zagreb indices, polycyclic aromatic hydrocarbon, benzenoid system

AMS Mathematics Subject Classification (2010): 05C05, 05C07, 05C90

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 to [1] for undefined term and notation.

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.

Recently, Furtula et al., in [2] introduced the reduced second Zagreb index, defined as

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

Recently, some new reduced indices were studied, for example, in [3, 4, 5, 6, 7].

The reduced first Zagreb index [8] of a graph G is defined as

$$RM_1(G)=\sum_{u\in V(G)}\left(d_G(u)-1\right)^2. \tag{1}$$

Motivated by the definition of the reduced first Zagreb index, we introduce the reduced modified first Zagreb index, reduced inverse degree index, reduced zeroth-order Randić index, induced F-index and generalized reduced first Zagreb index as follows:

The reduced modified first Zagreb index of a graph G is defined as

$$^{m}RM_1(G)=\sum_{u\in V(G)}\frac{1}{\left(d_G(u)-1\right)^2}. \tag{2}$$

The reduced inverse degree index of a graph G is defined as

$$RID(G)=\sum_{u\in V(G)}\frac{1}{d_G(u)-1}. \tag{3}$$

The reduced zeroth-order index of a graph G is defined as

$$RZ(G)=\sum_{u\in V(G)}\frac{1}{\sqrt{d_G(u)-1}}. \tag{4}$$

The reduced F-index of a graph G is defined as

$$RF(G)=\sum_{u\in V(G)}(d_G(u)-1)^3. \tag{5}$$

The generalized reduced first Zagreb index of a graph G is defined as

$$RM_1^a(G)=\sum_{u\in V(G)}(d_G(u)-1)^a. \tag{6}$$

where a is a real number.

Recently, many topological indices were studied, for example, in [9, 10, 11,12,13,14,15,16,17,18,19,20,21,22,23]; the modified first Zagreb index was studied in [24,25] and the F-index was studied in [26,27,28,29,30,31].

In this paper, some reduced Zagreb indices of polycyclic aromatic hydrocarbons and benezenoid systems are computed. For more information about polycyclic aromatic hydrocarbons and benzenoid systems see [32].

2. Results for polycyclic aromatic hydrocarbons

In this section, we focus on the chemical graph structure of the family of polycyclic aromatic hydrocarbons, denoted by PAH_n. The first three members of the family PAH_n are given in Figure 1.

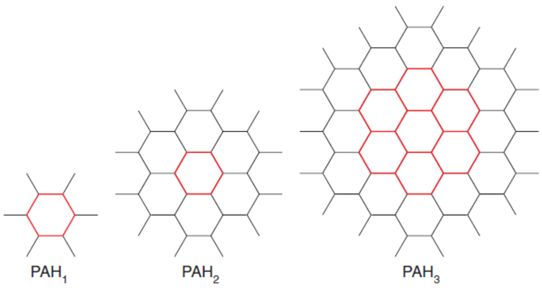

Figure 1:

Let $G = PAH_n$ be the chemical graph in the family of polycyclic aromatic hydrocarbons. By calculation, we obtain that G has $6n^2+6n$ vertices. In G, there are two types of vertices as follows:

$V_1 = \{u \in V(G) \mid d_G(u) = 1\}$, $|V_1| = 6n$.

$V_3 = \{u \in V(G) \mid d_G(u) = 3\}$, $|V_3| = 6n^2$.

In the following theorem, we compute the generalized reduced first Zagreb index of PAH_n.

Theorem 1. The generalized reduced first Zagreb index of the family of polycyclic aromatic hydrocarbons PAH_n is

$$RM_1^a\left(PAH_n\right) = 2^a \times 6n^2. \qquad (7)$$

Proof: Let $G = PAH_n$ be the chemical graph in the family of polycyclic aromatic hydrocarbons. From equation (6) and by cardinalities of the vertex partition of PAH_n, we have

$$RM_1^a\left(PAH_n\right) = \sum_{u \in V(G)} \left(d_G(u) - 1\right)^a .$$

$$= (1-1)^a 6n + (3-1)^a 6n^2$$

$$= 2^a \times 6n^2.$$

We obtain the following results by using Theorem 1.

Corollary 1.1. The reduced first Zagreb index of PAH_n is given by

$$RM_1(PAH_n)=24n^2.$$

Proof: Put $a = 2$ in equation (7), we get the desired result.

Corollary 1.2. The reduced modified first Zagreb index of PAH_n is given by

$${}^{m}RM_1\left(PAH_n\right) = \frac{3}{2}n^2.$$

Proof: Put $a = -2$ in equation (7), we get the desired result.

Corollary 1.3. The reduced inverse degree index of PAH_n is given by

$$RID(PAH_n) = 3n^2.$$

Proof: Put $a = -1$ in equation (7), we obtain the desired result.

Corollary 1.4. The reduced zeroth-order Randić index of PAH_n is given by

$$RZ\left(PAH_n\right) = \frac{6}{\sqrt{2}}n^2.$$

Proof: Put $a = -\frac{1}{2}$ in equation (7), we obtain the desired result.

Corollary 1.5. The reduced F-index of PAH_n is given by

$$RF(G) = 48n^2.$$

Proof: Put $a = 3$ in equation (7), we get the desired result.

3. Results for benzenoid systems

In this section, 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 presented in Figure 2.

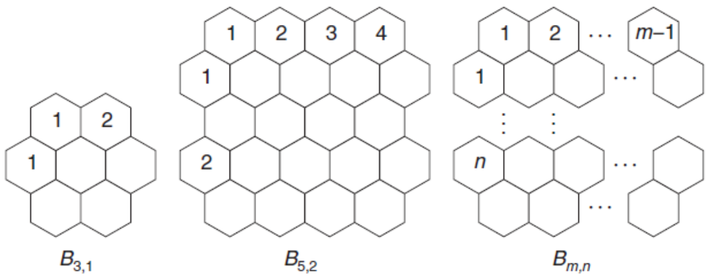

Figure 2:

Let $G = B_{m,\,n}$ be the chemical graph in the family of a jagged rectangle benzenoid system. By calculation, we obtain that G has $4mn+4m+2n-2$ vertices. In G, there are three types of vertices as follows:

$V_2 = \{u \in V(G) \mid d_G(u) = 2\}$, $\qquad |V_2| = 2m + 4n + 2$.
$V_3 = \{u \in V(G) \mid d_G(u) = 3\}$, $\qquad |V_3| = 4mn + 2m - 2n - 4$.

In the following theorem, we compute the generalized reduced first Zagreb index of $B_{m,\,n}$.

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

$$RM_1^a\left(B_{m,n}\right) = (2m+4n+2) + 2^a\,(4mn+2m-2n-4). \tag{8}$$

Proof: Let $G = B_{m,\,n}$ be the chemical graph in the family of a jagged rectangle benzenoid system. From equation (6) and by cardinalities of the vertex partition of $B_{m,n}$, we have

$$\begin{aligned} RM_1^a\left(B_{m,n}\right) &= \sum_{u \in V(G)} \left(d_G(u) - 1\right)^a \\ &= (2-1)^a\,(2m+4n+2) + (3-1)^a\,(4mn+2m-4n-4) \\ &= (2m+4n+2) + 2^a\,(4mn+2m-4n-4) \end{aligned}$$

We obtain the following results by using Theorem 2.

Corollary 2.1. The reduced first Zagreb index of $B_{m,n}$ is given by

$$RM_1(B_{m,n}) = 16mn + 10m - 4n - 14.$$

Proof: Put $a = 2$ in equation (8), we get the desired result.

Corollary 2.2. The reduced modified first Zagreb index of $B_{m,n}$ is given by

$$^{m}RM_1\left(B_{m,n}\right) = mn + \frac{5}{2}m - \frac{7}{2}n + 1.$$

Proof: Put $a = -2$ in equation (8), we get the desired result.

Corollary 2.3. The reduced inverse degree index of $B_{m,n}$ is given by

$$RID(B_{m,n}) = 2mn + 3m + 2n.$$

Proof: Put $a = -1$ in equation (8), we get the desired result.

Corollary 2.4. The reduced zeroth-order Randić index of $B_{m,n}$ is given by

$$RZ\left(B_{m,n}\right)=2\sqrt{2}mn+\left(2+\sqrt{2}\right)m+\left(4-\sqrt{2}\right)n+\left(2-\sqrt{2}\right).$$

Proof: Put $a=-\frac{1}{2}$ in equation (8), we obtain the desired result.

Corollary 1.5. The reduced F-index of $B_{m,n}$ is given by

$$RF(B_{m,n})=32mn+18m-12n-30.$$

Proof: Put $a = 3$ in equation (8), we get the desired result.

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REFERENCES

1. V.R.Kulli, *College Graph Theory*, Vishwa International Publications, Gulbarga, India (2012).
2. B.Furtula, I.Gutman and S.Ediz, On difference of Zagreb indices, *Discrete Appl. Math.*, 178 (2018) 83-88.
3. I.Gutman, B.Furtula and C.Elphick, Three new/old vertex degree based topological indices, *MATCH Commun. Math. Comput. Chem.,* 72 (2014) 617-682.
4. B.Horoldagva, L.Buyantoglokh and S.Dorjsembe, Difference of Zagreb indices and reduced second Zagreb index of cyclic graphs with cut edges, *MATCH Commun. Math. Comput. Chem.,* 78 (2017) 337-350.
5. V.R.Kulli, Reduced second hyper-Zagreb index and its polynomial of certain silicate networks, *Journal of Mathematics and Informatics,* (2018).
6. V.R.Kulli, General reduced second Zagreb index of certain networks, submitted.
7. V.R.Kulli, Some multiplicative reduced indices of certain nanostructures, submitted.
8. S.Ediz, On the reduced first Zagreb index of graphs, *Pacific Journal of Applied Mathematics,* 8(2) (2016) 99-102.
9. V.R.Kulli, On *K* indices of graphs, *International Journal of Fuzzy Mathematical Archive*, 10(2) (2016) 105-109.
10. V.R.Kulli, On *K*-edge index of some nanostructures, *Journal of Computer and Mathematical Sciences*, 7(7) (2016) 373-378.
11. V.R.Kulli, On *K* Banhatti indices and *K* hyper-Banhatti indices of *V*-Phenylenic nanotubes and nanotorus, *Journal of Computer and Mathematical Sciences,* 7(6) (2016) 302-307.
12. V.R.Kulli, General topological indices of circumcoronene series of benzenoid, *International Research Journal of Pure Algebra,* 7(5) (2017) 748-753.
13. V.R.Kulli, Computation of some Gourava indices of titania nanotubes, *Interational Journal of Fuzzy Mathematical Archive*, 12(2) (2017) 75-81.
14. V.R.Kulli, Computing Banhatti indices of networks, *International Journal of Advances in Mathematics*, 2018(1) (2018) 31-40.
15. V.R.Kulli, Some new fifth multiplicative Zagreb indices of PAMAM dendrimers, *Journal of Global Research in Mathematics,* 5(2) (2018) 82-86.

16. V.R.Kulli, Multiplicative connectivity Banhatti indices of dendrimer nanostars, *Journal of Chemistry and Chemical Sciences*, 8(6) (2018) 964-973.
17. V.R.Kulli, Connectivity Revan indices of chemical structures in drugs, *International Journal of Engineering Sciences and Research Technology,* 7(5) (2018).
18. V.R.Kulli, On augmented reverse index and its polynomial of certain nanostar dendrimers, *International Journal of Engineering Sciences and Research Technology,* 7(8) (2018) 237-243.
19. V.R.Kulli, On two arithmetic-geometric Banhatti indices of certain dendrimer nanostars, *International Journal of Fuzzy Mathematical Archive,* 16(1) (2018) 7-12.
20. V.R.Kulli, Computation of arithmetic-geometric Revan indices of certain benzenoid systems, *Journal of Global Research in Mathematical Archives*, (2018).
21. V.R.Kulli, Computing two arithmetic-geometric reverse indices of certain networks, *International Research Journal of Pure Algebra*, (2018).
22. V.R.Kulli and M.H.Akhbari, Multiplicative atom bond connectivity and multiplicative geometric-arithmetic indices of dendrimer nanostars, *Annals of Pure and Applied Mathematics*, 16(2) (2018) 429-436.
23. V.R.Kulli, B.Chaluvaraju and H.S.Baregowda, *K*-Banhatti and *K* hyper-Banhatti indices of windmill graphs, *South East Asian J. of Math. and Math. Sci*, 13(1) (2017) 11-18.
24. V.R.Kulli, Some topological indices of certain nanotubes, *Journal of Computer and Mathematical Sciences*, 8(1) (2017) 1-7.
25. V.R.Kulli, General topological indices of circumcoronene series of benzenoid, *International Research Journal of Pure Algebra*, 7(5)(2017) 748-753.
26. V.R.Kulli, Computing F-reverse index and F-reverse polynomial of certain networks, *International Journal of Mathematical Archive,* 9(8) (2018).
27. V.R Kulli, Edge version of *F*-index, general sum connectivity index of certain nanotubes, *Annals of Pure and Applied Mathematics*, 14(3) (2017) 449-455.
28. V.R.Kulli, General Zagreb polynomials and F-polynomial of certain nanostructures, *International Journal of Mathematical Archive,* 8(10) (2017) 103-109.
29. V.R.Kulli, *F*-index and reformulated Zagreb index of certain nanostructures, *International Research Journal of Pure Algebra*, 7(1) (2017) 489-495.
30. V.R.Kulli, Computing the F-ve-degree index and its polynomial of dominating oxide and regular triangulate oxide networks, *International Journal of Fuzzy Mathematical Archive*, 16(1) (2018) 1-6.
31. V.R.Kulli, Computation of F-reverse and modified reverse indices of some nanostructures, *Annals of Pure and Applied Mathematics*, 18(1) (2018) 37-43.
32. V.R.Kulli, B.Stone, S.Wang and B.Wei, Generalized multiplicative indices of polycyclic aromatic hydrocarbons and benzenoid systems, *Z. Naturforsch*, 72(6)a (2017) 573-576.