ISSN 2229-5518

The Multiplicative Zagreb Eccentricity Index of Polycyclic Aromatic Hydrocarbon (PAHk)

Mohammad Reza Farahani, Muhammad Kamran Jamil, M.R. Rajesh Kanna, R. Pradeep Kumar

Abstract—First and second Zagreb indices are defined as $M_1(G)=\sum_{v\in V(G)} d(v)^2$ and $M_2(G)=\sum_{uv\in E(G)} d(u)d(v)$, respectively. The first and second multiplicative Zagreb eccentricity indices of G are defined as $\prod E_1(G)=\prod_{v\in V(G)} \varepsilon(v)^2$ and $\prod E_2(G)=\sum_{uv\in E(G)} \varepsilon(u)\varepsilon(v)$, respectively. In this paper, we compute the first multiplicative Zagreb index of Polycyclic aromatic hydrocarbons (PAHk) by using the cut-method and ring cut method.

Index Terms—Eccentric, Eccentricity, Zagreb indices, ring cut method, polycyclic aromatic hydrocarbon.

1 Introduction

Let $G(V_G,E_G)$ be a simple connected graph with vertex set V_G and edge set E_G, the number of elements in V_G is called the *order* of the graph G and the number of elements in E_G is called the *size* of the graph G. For a vertex $v\in V(G)$, the number of vertices adjacent to the vertex v is called the *degree* of v, denote as $d(v)$. For the vertices $u,v\in V(G)$, the length of the shortest path connecting u and v is called the *distance* between u and v, denoted as $d(u,v)$. The maximum distance between v and any other vertex of G is called the *eccentricity* of v, denoted as $\varepsilon(v)$. The maximum and minimum eccentricity of G is called the *diameter* and *radius*, respectively, of G.

A topological index is a real number related to a molecular graph without relying on the pictorial representation or labeling of graph. There are many vertex-degree-based and vertices distance based topological indices be defined in chemical graph theory. The first and second Zagreb indices M_1 and M_2 are the oldest and extensively studied vertex-based-topological indices defined by Gutman and Trinajstić [1,3]. They are defined as

$$M_1(G)=\sum_{v\in V(G)} d(v)^2$$

$$M_2(G)=\sum_{uv\in E(G)} d(u)d(v)$$

The multiplicative variant of Zagreb indices was introduced by Todeschini et. al. [2,5]

$$\prod\nolimits_1(G)=\prod_{v\in V(G)} d(v)^2$$

$$\prod\nolimits_2(G)=\prod_{uv\in E(G)} d(u)d(v)$$

Recently, the first and second Zagreb eccentricity indices M_1^* and M_2^* of a connected G have been introduced by Ghorbani et. al. [4] and Vukičević et. al. [6] as the revised version of the Zagreb indices. They are defined as:

$$M_1^*(G)=\sum_{v\in V(G)} \varepsilon(v)^2$$

$$M_2^*(G)=\sum_{uv\in E(G)} \varepsilon(u)\varepsilon(v)$$

Nilanjan [7] introduced the multiplicative Zagreb eccentricity index and defined as:

$$\prod E_1(G)=\prod_{v\in E(G)} \varepsilon(v)^2$$

Reader interested in history and more results about Zagreb indices see [7-16].

Polycyclic Aromatic Hydrocarbons (PAHk) are a group of over 100 different chemicals that are formed during the incomplete burning of coal, oil and gas, garbage, or other organic substances like tobacco or charbroiled meat. PAHk are usually found as a mixture containing two or more of these compounds, such as soot. For detailed study see [17-19].

- Mohammad Reza Farahani is from Department of Applied Mathematics of Iran University of Science and Technology (IUST), Narmak, Tehran 16844,Iran. E-mail: MrFarahani88@Gmail.com
- Muhammad Kamran Jamil is a faculty member of Department of Mathematics, Riphah Institute of Computing and Applied Sciences (RICAS), Riphah International University, Lahore, Pakistan. E-mail: m.kamran.sms@gmail.com
- M.R. Rajesh Kanna is a faculty member of Department of Mathematics, Maharani's Science College for Women, Mysore- 570005. India. E-mail: mr.rajeshkanna@gmail.com
- R. Pradeep Kumar is fromDepartment of Mathematics, The National Institute of Engineering, Mysuru- 570008, India.
- pradeepr.mysore@gmail.com

ISSN 2229-5518

2 Main Results and Discussion

In this section we computed the multiplicative Zagreb eccentricity index of Polycyclic Aromatic Hydrocarbons (PAHk). The first members of the hydrocarbon family are shown in Figure 1. A general representation of PAHk is shown in Figure 2. PAHk has $6k^2+6k$ vertices.

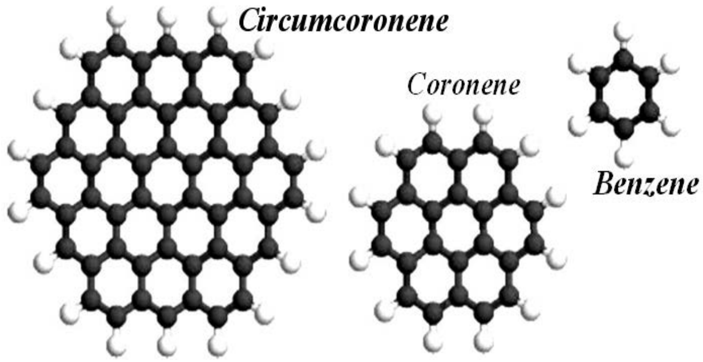

Figure 1. The first three members of PAHk family.

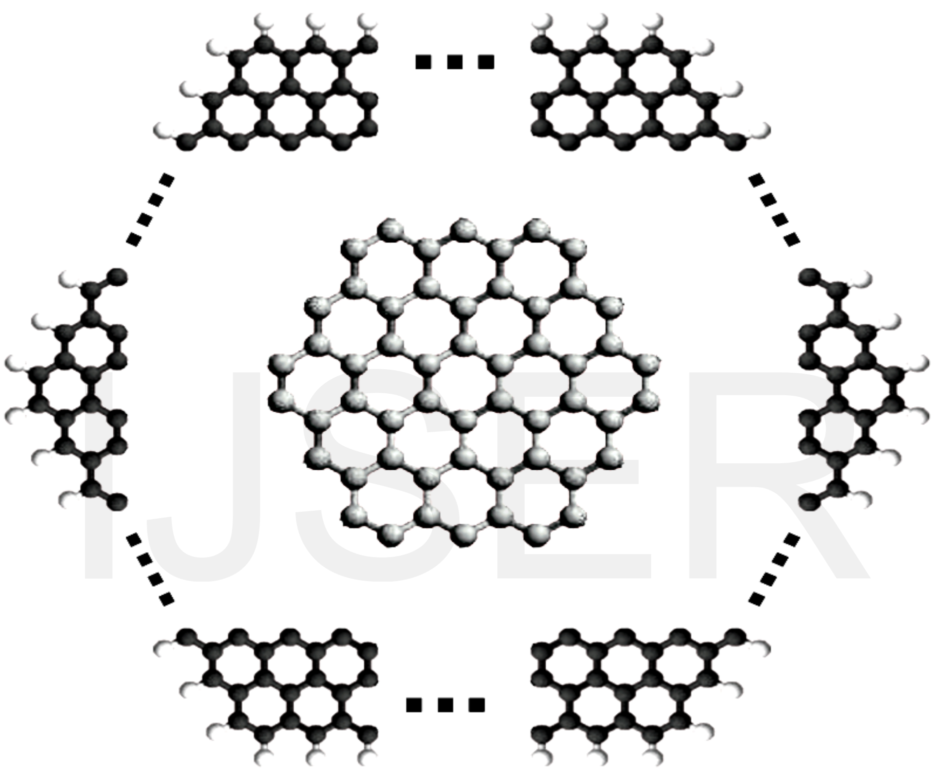

Figure 2. A general representation of polycyclic aromatic hydrocarbon (PAHk).

Theorem: Let the graph of Polycyclic aromatic hydrocarbon (PAHk). The multiplicative Zagreb eccentricity index of PAHk is equal to

$$\prod E_1\left(PAH_k\right) = \left(14k+1\right)^{12k} \prod_{i=1}^{k} \left(\left(2k+2i-2\right)^{12(i-1)}\right)\left(\left(2k+2i-1\right)^{12i}\right)$$

Proof. To obtain the desired result, we used the *Cut Method* and *Ring cut Method*. The Ring cut method divides all vertices of a graph G into some partitions with similar mathematical and topological properties. For further detail see [20-22]. We will denote the vertices of degree three with γ and β, and the vertices with degree one with α see Figure 3. Clearly, the set of vertices is $V\left(PAHk\right) = \{\alpha_{z,l}, \beta^i_{z,l}, \gamma^i_{z,j} \mid i=1,\cdots,k;\ j\in Z_i; l \in Z_{i-1}; z \in Z_6\}$ where $Z_i = \{1,\cdots,i\}$.

Ring cuts divide the vertex set in some partitions, such that ith ring cut contain *12i-6* vertices which are $\beta^i_{z,j}$ and $\gamma^i_{z,j}\left(i=2,\cdots,k; z\in Z_6, j \in Z_i\right)$. From ring cuts we also notice that $d(\beta^i_{z,l},\beta^k_{z,l}) = d(\gamma^i_{z,j},\gamma^k_{z,j})=2(k-i)$. From these results and Figure 3, we found that

- For all vertices $\alpha_{z,j}$ of PAH_k $\left(j \in Z_k, z \in Z_6\right)$

$$\varepsilon(\alpha_{z,j}) = \underbrace{d(\alpha_{z,j},\gamma^k_{z,j})}_{1} + \underbrace{d(\gamma^k_{z,j},\gamma^k_{z',j'})}_{4k-1} + \underbrace{d(\gamma^k_{z',j'},\alpha_{z',j'})}_{1} = 4k+1$$

- For all vertices $\beta^i_{z,j}$ of PAH_k $(\forall i=1,..,k;\ z\in\mathbb{Z}_6,\ j\in\mathbb{Z}_{i-1})$

$$\varepsilon(\beta^{i}_{z,j}) = \underbrace{d(\beta^{i}_{z,j},\beta^{i}_{z+3,j})}_{4i-3} + \underbrace{d(\beta^{i}_{z+3,j},\gamma^{k}_{z+3,j})}_{2(k-i)+1} + \underbrace{d(\gamma^{k}_{z+3,j},\alpha_{z+3,j})}_{1}$$

=2k+2i-1

- For all vertices $\gamma^{i}_{z,j}$ of PAH_n ($\forall i=1,..,k;\ z\in\mathbb{Z}_6,\ j\in\mathbb{Z}_i$)

$$\varepsilon(\gamma^{i}_{z,j}) = \underbrace{d(\gamma^{i}_{z,j},\gamma^{i}_{z+3,j})}_{4i-1} + \underbrace{d(\gamma^{i}_{z+3,j},\gamma^{k}_{z+3,j})}_{2(k-i)} + \underbrace{d(\gamma^{k}_{z+3,j},\alpha_{z+3,j})}_{1}$$

=2(k+i)

From the above calculation we are able to find the multiplicative Zagreb eccentricity index of PAHk.

$$\prod E_1(G) = \prod_{v\in E(G)} \varepsilon(v)^2$$

$$= \prod_{\alpha_{z,j}\in V(PAH_k)} \varepsilon^2(\alpha_{z,j}) \times \prod_{\beta^{i}_{z,j}\in V(PAH_k)} \varepsilon^2(\beta^{i}_{z,j}) \times \prod_{\gamma^{i}_{z,j}\in V(PAH_k)} \varepsilon^2(\gamma^{i}_{z,j})$$

$$= \prod_{z=1}^{6}\left(\prod_{j=1}^{k}\varepsilon^2(\alpha_{z,j})\right)\times\prod_{z=1}^{6}\left(\prod_{i=2}^{k}\prod_{j=1}^{i}\varepsilon^2(\beta^{i}_{z,j})\right)\times\prod_{z=1}^{6}\left(\prod_{i=1}^{k}\prod_{j=1}^{i}\varepsilon^2(\gamma^{i}_{z,j})\right)$$

$$= \prod_{j=1}^{k}\left(\varepsilon^2(\alpha_{z,j})\right)^6 \times \prod_{i=2}^{k}\prod_{j=1}^{i}\left(\varepsilon^2(\beta^{i}_{z,j})\right)^6$$

$$\times \prod_{i=1}^{k}\prod_{j=1}^{i}\left(\varepsilon^2(\gamma^{i}_{z,j})\right)^6$$

$$= \left((4k+1)^{(k)}\right)^{12} \times \left(\prod_{i=2}^{k}\left((2k+2i-2)^{(i-1)}\right)^{12}\right)$$

$$\times \left(\prod_{i=1}^{k}\left((2k+2i-1)^{(i)}\right)^{12}\right)$$

$$= (14k+1)^{12k} \prod_{i=1}^{k}\left((2k+2i-2)^{12(i-1)}\right)\left((2k+2i-1)^{12i}\right)$$

Which is the required result, hence proof.■

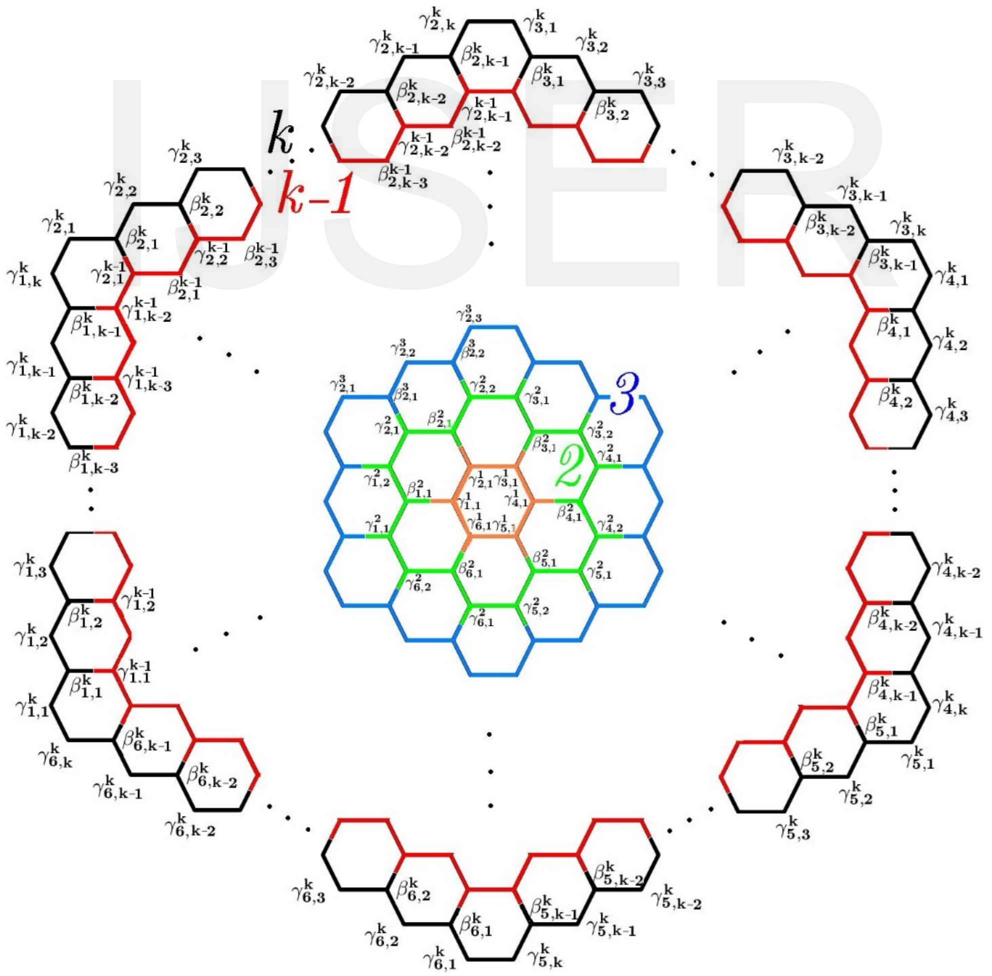

Figure 3. General vertex and ring cut representation of Hk.

REFERENCES

[1] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals, Total π electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* 17 (1972) 13-19.

[2] R. Todeschini, V. Consonni, New local vertex invariants and molecular descriptors based on functions of the vertex degree, *MATCH Commun. Comput. Chem.*, 64 (2010) 359-372.

[3] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* 50 (2004) 83-92.

[4] M. Ghorbani, M. A. Hosseinzadeh, A new version of Zagreb indices, *Filomat* 26 (2012) 93-100.

[5] R. Todeschini, D. Ballabio, V. Consonni, Novel molecular descriptors based on functions of the vertex degrees, in: I. Gutman, B. Furtula (Eds), Novel Molecular structure descriptors- Theory and Applications I, Univ. Kragujevac, Kragujevac, (2010) 73-100.

[6] D. Vukicevic, A. Graovac, Note on the comparison of the first and second normalized Zagreb eccentricity indices, *Acta. Chim. Solv.*, 57 (2010) 524-528.

[7] M.H. Khalifeh, H. Yousefi–Azari, A. R. Ashrafi, The first and second Zagreb indices of graph operations, *Discr. Appl. Math.* 157 (2009) 804–811.

[8] I. Gutman, Multiplicative Zagreb indices of trees, Bull. Internat. Math. Virt. Inst., 1 (2011),13-19.

[9] K. Xu, H. Hua, A united approach to extremal multiplicative Zagreb indices for trees, unicyclic and bicyclic graphs, MATCH Commun. Math. Comput. Chem., 68 (2012) 241-256.

[10] J. Liu, Qianhong Zhang, Sharp Upper Bounds for Multiplicative Zagreb Indices, MATCH Commun. Math. Comput. Chem., 68 (2012) 231-240.

[11] T. Reti and I. Gutman, Relations between Ordinary and Multiplicative Zagreb Indices, Bull. Internat. Math. Virt. Inst., 2 (2012), 133-140.

[12] M. K. Jamil, I. Tomescu, N. Akhter, Extremal degree-product indices of graphs with fixed number of pendant vertices and cyclomatic number, International Letters of Chemistry, Physics and Astronomy 59 (2015) 53-61.

[13] M.R. Farahani. Multiplicative Versions of Zagreb indices of $TUSC_4C_8(S)$. Journal of Chemistry and Materials Research, 2(2), 2015, 67-70.

[14] M.R. Farahani. On Multiple Zagreb indices of Dendrimer Nanostars. International Letters of Chemistry, Physics and Astronomy. 52, (2015), 147-151.

[15] M.R. Farahani. A New Version of Zagreb Index of Circumcoronene Series of Benzenoid. *New. Front. Chem.* (2014). 23(2). 141-147.

[16] I. Gutman, M. K. Jamil, N. Akhter, Graphs with fixed number of pendent vertices and minimal first Zagreb index, Transactions on Combinatorics, 4 (1) (2015) 43-48.

[17] U.E. Wiersum, L.W. Jenneskens. Gas Phase Reactions in Organic Synthesis, (Ed.: Y. Valle. e), *Gordon and Breach Science Publishers*, Amsterdam. The Netherlands, 1997, 143–194.

[18] C.W. Bauschlicher, Jr, E.L.O. Bakes, *Chem. Phys.* 2000, *262*, 285-291

[19] S. E. Stein, R. L. Brown, *J. Am. Chem. Soc.* 1987, *109*, 3721-3729.

[20] M.R. Farahani. A New Version of Zagreb Index of Circumcoronene Series of Benzenoid. *Chemical Physics Research Journal*. 6(1), 27-33, (2013).

[21] M.R. Farahani, *Eccentricity Version of Atom-Bond Connectivity Index of Benzenoid Family $ABC_5(H_k)$. World Applied Sciences Journal*, 21(9), (2013), 1260-126.

[22] M.R. Farahani. Computing Eccentricity Connectivity Polynomial of Circumcoronene Series of Benzenoid H_k by Ring-Cut Method. *Annals of West University of Timisoara-Mathematics and Computer Science.* 51(2), (2013), 29–37.