GENERAL ZAGREB INDEXES OF A HYDROCARBON MOLECULAR GRAPH "POLYCYCLIC AROMATIC HYDROCARBONS (PAHK)"

YINGFANG LI[1], LI YAN[2] MUHAMMAD KAMRAN JAMIL[3] AHMAD N. AL-KENANI[4] AND MOHAMMAD REZA FARAHANI[5]*

1: School of Engineer, Honghe University, Mengzi 661100, China

E Mail: 1013747460@qq.com

2: School of Engineer, Honghe University, Mengzi 661100, China

E Mail: yanli_uoh@163.com

3: Department of Mathematics, Riphah Institute of Computing and Applied Sciences (RICAS), Riphah International University, Lahore, Pakistan

E Mail: m.kamran.sms@gmail.com

4: Department of Mathematics, King Abdulaziz University, Jeddah, Saudi Arabia.

E Mail: aalkenani10@hotmail.com

5: Department of Applied Mathematics of Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran

E Mail: MrFarahani88@Gmail.com; Mr_Farahani@Mathdep.iust.ac.ir

ABSTRACT

The *Zagreb index* is one of the most useful and thoroughly studied topological indexes. For a graph *G*, it is defined as $M_1(G) = \sum_{v \in V(G)} d(v)^2$. The *general Zagreb index* is defined as

$M_1^\alpha(G) = \sum_{v \in V(G)} d(v)^\alpha$, α is any real number. In this article, we computed the general Zagreb index of the *Polycyclic aromatic hydrocarbons (PAH$_k$)*.

Keywords: Topological index, Molecular graphs, Chemical structures Polycyclic Aromatic Hydrocarbon (PAH$_k$), Circumcoronene series of Benzenoid.

INTRODUCTION

Let *G(V,E)* be a simple connected graph, where *V* and *E* represent the set of vertices and the set of edges. The number of elements in *V* is called the *order* of the graph *G* and the number of elements in *E* is called the *size* of the graph *G*. The number of vertices adjacent to the vertex $v \in V$ is called the *degree* of *v* and is denoted as *d(v)*.

A *topological index* (molecular structure descriptor) is a numerical value related with chemical constitution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. A *molecular graph* is a simple graph representing the carbon atom skeleton of an organic molecule. In molecular graphs, the vertices represents the carbon atoms and the edges represents the carbon-carbon bonds. Usually, the hydrocarbons are considered as molecular graphs. *Polycyclic aromatic hydrocarbons (PAH_k)* are composed of two or more benzene (aromatic) rings which are fused together when a pair of carbon atoms is shared between them. The resulting structure is a molecule where all carbon and hydrogen atoms lie in one plane. PAH_k are formed during the incomplete burning of coal, gas, oil, garbage, wood, or other organic substances. First three members of this family is shown in Fig. 1.

The first degree based topological index was proposed in 1975 by *Milan Randić*. He defined this topological index as;

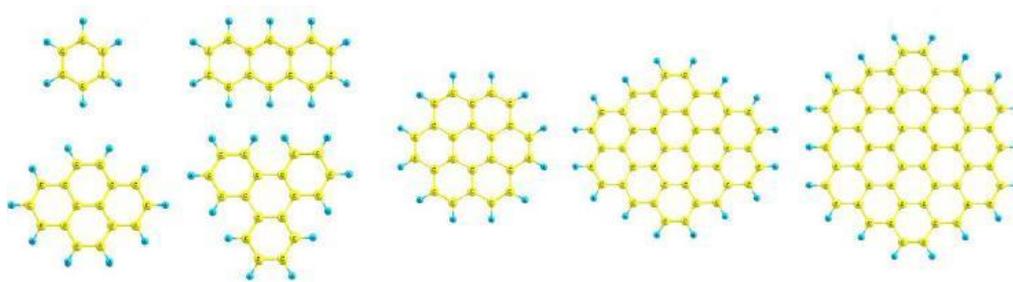$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$$

Figure 1: First three members of the Polycyclic aromatic hydrocarbons family

The Randić index is the most studied and most popular among all topological indices. A lot of papers and a few books are dedicated to this graph invariant [1-8].

Bollobás and *Erdös* [9] defined the *general Randić index* as follows

$$R_\alpha(G) = \sum_{uv \in E(G)} \left(d(u)d(v)\right)^\alpha$$

where α is a real number. For further history and details of general Randić index see [10-13].

Zhou et. al. [14] replaced the term $d(u)d(v)$ by $d(u)+d(v)$ in Randić index and introduced the *sum-connectivity index* as

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)+d(v)}}$$

In 2010, the concept of sum-connectivity index was extend to the *general sum-connectivity index* in [15].

$$\chi_\alpha(G) = \sum_{uv \in E(G)} \left(d(u)+d(v)\right)^\alpha$$

where α is any real number. Several properties of the general sum-connectivity index were discussed in [16-19].

The first and second *Zagreb indices* are among the oldest and most famous

topological indices. These topological indices were introduced by *Gutman* and Trinajstić [20]. These are defined as

$$M_1(G) = \sum_{v \in V(G)} d(v)^2$$
$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

A lot of research papers have published on these important topological indices few of them are [21-23].

In 2005, *Li* and *Zheng* [24] proposed the *first general Zagreb index*

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

where α is any real number. Some results on first general Zagreb index can be seen in [25,26].

In this paper, we computed the first general Zagreb index of the *Polycyclic aromatic hydrocarbons (PAH$_k$)*.

RESULTS

A general representation of the polycyclic aromatic hydrocarbons (PAH$_k$) is shown in Fig. 2. The outer layers are *Hydrogen* atoms and all the inner are *Carbon* atoms. There are $6k^2$ Carbon atoms and $6k$ Hydrogen atoms. So, a PAH$_k$ structure contains $6k^2+6k$ atoms and there are $9k^2+3k$ bonds between Carbon-

Carbon and Carbon-Hydrogen atoms. Many of topological indices of these important hydrocarbons have found [27-32]. In the continual of this, we computed the first general Zagreb index of polycyclic aromatic hydrocarbons.

Theorem: Let the graph of the *Polycyclic aromatic hydrocarbons (PAH_k)*, the general Zagreb index of Polycyclic aromatic hydrocarbons is as

$$M_1^\alpha (PAH_k) = \begin{cases} 6k(9k+1); \; for\, \alpha = 2 \\ 6k(27k+1); \; for\, \alpha = 3 \\ 2k(k+3); \; for\, \alpha = -1 \end{cases}$$
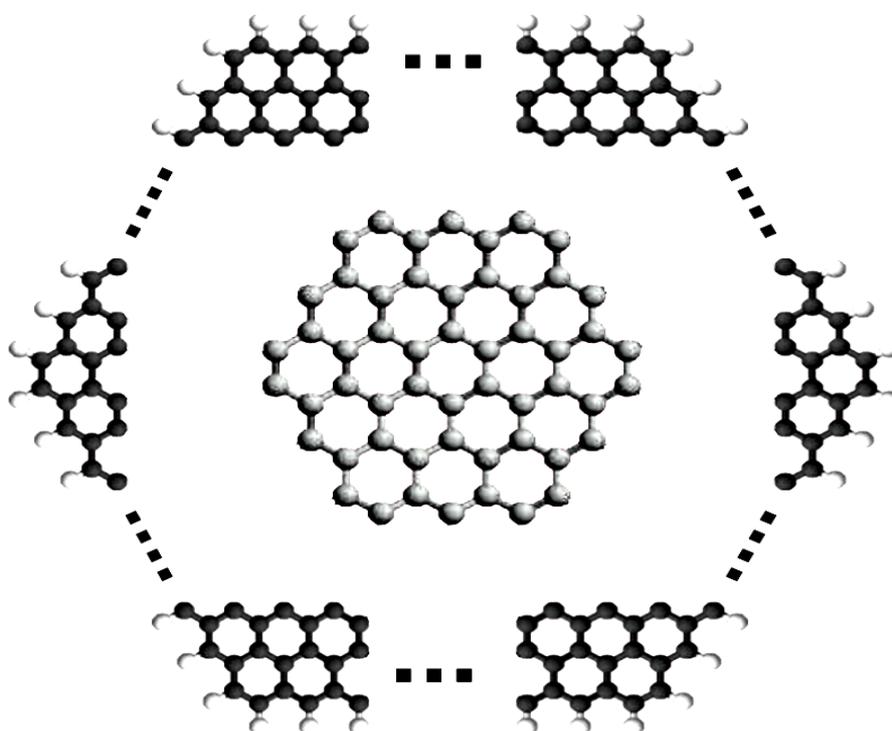

Figure 2: A general representation of the Polycyclic aromatic hydrocarbons

Proof. From Fig. 2, we can notice that in the structure of Polycyclic aromatic hydrocarbons (PAH_k) all the Carbons atoms have degree *3* and all the Hydrogen atoms have degree 1. So,

$$M_1^\alpha (PAH_k) = \sum_{v \in V(PAH_k)} d(v)^\alpha$$

$$= \sum_{c \in V(PAH_k)} d(c)^\alpha + \sum_{h \in V(PAH_k)} d(h)^\alpha$$

$$= \sum_{c \in V(PAH_k)} 3^{\alpha} + \sum_{h \in V(PAH_k)} 1^{\alpha}$$

$$= 6k^2 \cdot 3^{\alpha} + 6k \cdot 1$$

For $\alpha = 2$, we have

$$M_1^2(PAH_k) = 6k(3^2 k + 1)$$

For $\alpha = 3$, we have

$$M_1^3(PAH_k) = 6k(3^3 k + 1)$$

For $\alpha = -1$, we have

$$M_1^{-1}(PAH_k) = 2k(k + 3)$$

So, we have

$$M_1^{\alpha}(PAH_k) = \begin{cases} 6k(9k+1); \ for \ \alpha = 2 \\ 6k(27k+1); \ for \ \alpha = 3 \\ 2k(k+3); \ for \ \alpha = -1 \end{cases}$$

which is the required result.∎

REFERENCES

[1] M. Randić, J. Am. Chem. Soc. 97 (1975) 6609.

[2] L. B. Kier and L. H. Hall, Molecular Connectivity in Chemistry and Drug Research, Academic Press, New York, 1976.

[3] L. B. Kier and L. H. Hall, Molecular Connectivity in Structure-Activity Analysis, Wiley, New York, 1986.

[4] X. Li and I. Gutman, Mathematical Aspects of Randić-Type Molecular Structure Descriptors, Univ. Kragujevac, Kragujevac,2006.

[5] I. Gutman and B. Furtula (Eds.), Recent Results in the Theory of Randić Index, Univ. Kragujevac, Kragujevac, 2008.

[6] M. Randić, MATCH Commun. Math. Comput. Chem. 59 (2008) 5.

[7] M. Randić, J. Mol. Graphics Modell. 20 (2001) 19.

[8] X. Li and Y. Shi, MATCH Commun. Math. Comput. Chem. 59 (2008) 127.

[9] B. Bollobás, P. Erdös, Graphs of extremal weights, Ars Combi., 50 (1998) 225-233.

[10] L. Clark, I. Gutman, The exponent in the general Randić index, J. Math. Chem., in press.

[11] L. H. Clark, J. W. Moon, On the general Randić index for certain families of trees, Ars Combin. 54 (2000), 223-235.

[12] Y. Hu, X. Li and Y. Yuan, Trees with minimum general Randić index, *MATCH Commun. Math. Comput. Chem.* 52 (2004), 119–128.

[13] Y. Hu, X. Li and Y. Yuan, Trees with maximum general Randić index, *MATCH Commun. Math. Comput. Chem.* 52 (2004), 129–146.

[14] B. Zhou, N. Trinajstić, On a novel connectivity index, J. Math. Chem., 46 (2009) 1252-1270.

[15] B. Zhou, N. Trinajstić, On general sum-connectivity index, J. Math. Chem., 47 (2010) 210-218.

[16] Z. Du, Bo Zhou, N. Trinajstić, On the general sum-connectivity index of trees, Applied Mathematics Letters, 24 (2011) 402-405.

[17] I. Tomescu, M. Arshad, On the general sum-connectivity index of connected unicyclic graphs with k pendant vertices, Discr. Appl. Math., 181 (2015) 306-309.

[18] I. Tomescu, M. Arshad, M.K. Jamil, Extremal topological indices for graphs of given connectivity, Filomat, 29:7 (2015) 1639-1643.

[19] I. Tomescu, M.K. Jamil, Maximum general sum-connectivity index for trees with given independence number, MATCH Commun. Math. Comput. Chem., 72 (2014) 715-722.

[20] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals, Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett., 17 (1972) 535-538.

[21] Braun, A. Kerber, M. Meringer, C. Rucker, Similarity of molecular descriptors: the equivalence of Zagreb indices and walk counts, MATCH Commun. Math. Comput. Chem., 54 (2005) 163-176.

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

[23] N. Akhter, M.K. Jamil, I. Tomescu, Extremal first and second Zagreb indices of apex trees, U. P. B. Sci. Bull., Series A, to be appear.

[24] X. Li, J. Zheng, A unified approach to the extremal trees for different

indices, MATCH Commun. Math. Comput. Chem. 54 (2005) 195-208.

[25] H. Zhang and S. Zhang, Unicyclic graphs with the first three smallest and largest first general Zagreb index, *MATCH Commun. Math. Comput. Chem.* 55 (2006), 427–438.

[26] S. Zhang, W. Wang and T.C. E. Cheng, Bicyclic graphs with the first three smallest and largest values of the first general Zagreb index, *MATCH Commun. Math. Comput. Chem.* 55 (2006), 579–592.

[27] M.K. Jamil, M.R. Farahani, M.R. Rajesh Kanna, Fourth geometric arithmetic index of polycyclic aromatic hydrocarbons (PAH$_k$), The Pharmaceutical and Chemical Journal, 2016, 3(1) 94-99.

[28] M.R. Farahani, H.M. Rehman, M.K. Jamil, D.W. Lee, Vertex version of PI index of polycyclic aromatic hydrocarbons (PAH$_k$), The Pharmaceutical and Chemical Journal,2016, 3(1) 138-141.

[29] M.K. Jamil, M.R. Farahani, M. Imran, M. A. Malik, Computing eccentric version of second Zagreb index of Polycyclic aromatic hydrocarbons (PAH$_k$), Applied

Mathematics and Nonlinear Sciences, 2016 1(1) 247-251.

[30] M.R. Farahani, M.K. Jamil, M.R. R. Kanna, R. P. Kumar, Computation on the fourth Zagreb index of polycyclic aromatic hydrocarbons (PAH$_k$), Journal of Chemical and Pharmaceutical Research, 2016 8(4) 41-45.

[31] M.K. Jamil, M.R. Farahani, M.R.R. Kanna, R.P. Kumar, The second Zagreb eccentricity index of polycyclic aromatic hydrocarbons (PAH$_k$), Journal of Chemical and Pharmaceutical Research, 2016 8(4) 80-83.

[32] D. W. Lee, M.K. Jamil, M.R. Farahani, H.M. Rehman, The Ediz eccentric connectivity index of polycyclic aromatic hydrocarbons (PAH$_k$), Sch. J. Eng. Tech., 2016 4(3) 148-152.