Journal of Informatics and Mathematical Sciences
Vol. 10, Nos. 1 & 2, pp. 153–160, 2018
ISSN 0975-5748 (online); 0974-875X (print)
Published by RGN Publications

http://www.rgnpublications.com

http://dx.doi.org/10.26713/jims.v10i1-2.545

Research Article

About Atom Bond Connectivity and Geometric-Arithmetic Indices of Special Chemical Molecular and Nanotubes

Mohamad Nazri Husin[1], Mohammad Reza Farahan[2,*] and Waqas Nazeer[3]

[1] *School of Informatics and Applied Mathematics of University Malaysia, Terengganu, 21030 Kuala Terengganu, Malaysia*
[2] *Department of Applied Mathematics of Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran*
[3] *Division of Science and Technology, University of Education, Lahore 54000, Pakistan*
***Corresponding author:** mrfarahani88@gmail.com, mr_farahani@mathdep.iust.ac.ir

Abstract. Among topological descriptors connectivity indices are very important and they have a prominent role in chemistry. Two useful of them are the *geometric-arithmetic* (GA) and atom-bond connectivity (ABC) indices and are defined as $GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$ and $ABC(G) = \sum_{e=uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}$, in which d_u and d_v are the degrees of the vertices u and v, respectively. In this paper we compute these connectivity topological indices for a special chemical molecular graph "$Cas(C)$-$CaR(C)[m,n,p]$ Nanotubes Junction" are given. The $Cas(C)$-$CaR(C)[m,n,p]$ Nanotubes Junction is a new nano-structure that was defined by M.V. Diudea, on based the new graph operations (Leapfrog Le and Capra Ca) on the cycle graph C_n.

Keywords. Molecular graph; Nanotubes; geometric-arithmetic (GA) index, atom-bond connectivity (ABC) index

MSC. 05A15; 05C05; 05C12; 05C50

Received: December 20, 2016 **Accepted:** March 13, 2017

Copyright © 2018 Mohamad Nazri Husin, Mohammad Reza Farahan and Waqas Nazeer. *This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.*

1. Introduction

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. In chemical graphs, the vertices and edges of a graph also correspond to the atoms and bonds of the molecular graph, respectively. If e is an edge/bond of G, connecting the vertices/atoms u and v, then we write $e = uv$ and say "u and v are adjacent" [16–27]. The graph G is said to be connected, if for every vertices u and v in $V(G)$ there exists a path connecting u and v.

Chemical graph theory is an important branch of graph theory, such that there exits many topological indices in it. The topological indices of the graph G are a number relation to the structure of the graph G and are invariant on the automorphism of the graph. The simplest topological indices are the number of vertices, the number of edges and degree of a vertex v of the graph G and we denoted by n, m and d_v, respectively. The degree of a vertex v is the number of vertices joining to v and the distance $d(u,v)$ in a graph is the number of edges in a shortest path connecting them.

One of the oldest topological indices is the *Wiener index* $W(G)$, introduced by the chemist *Harold Wiener* [27] in 1947. It is defined as the sum of topological distances $d(u,v)$ between any two atoms in the molecular graph

$$W(G) = \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} d(u,v).$$

Let G be a (molecular) graph with vertex and edge sets being denoted by $V(G)$ and $E(G)$, respectively. B. Furtula et al. introduced *Atom-Bond Connectivity index* (ABC) and *Geometric-Arithmetic index* (GA) [16, 25]. These indices are based on degrees of vertices and defined as follow, respectively.

$$ABC(G) = \sum_{e=uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}},$$

$$GA(G) = \sum_{e=uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v},$$

where d_u and d_v are the degrees of the vertices u and v, respectively. In all parts of this paper, our notation is standard and mainly taken from standard books of chemical graph theory [6–27].

2. Main Results

In this paper, we investigate the above presented topological Connectivity indices in a family of special chemical molecular graphs "$Cas(C)$-$CaR(C)[m,n,p]$ Nanotubes Junction" (see Figure 1).

The $Cas(C)$-$CaR(C)[m,n,p]$ Nanotubes Junction is a new nano-structure that was defined by M.V. Diudea [1], on based the new graph operations on the cycle graph C_n, namely: Leapfrog Le and Capra Ca. Some examples of graph operations (Leapfrog Le and Capra Ca) are shown in Figure 2 and Figure 3 and readers can see the references [2–15].

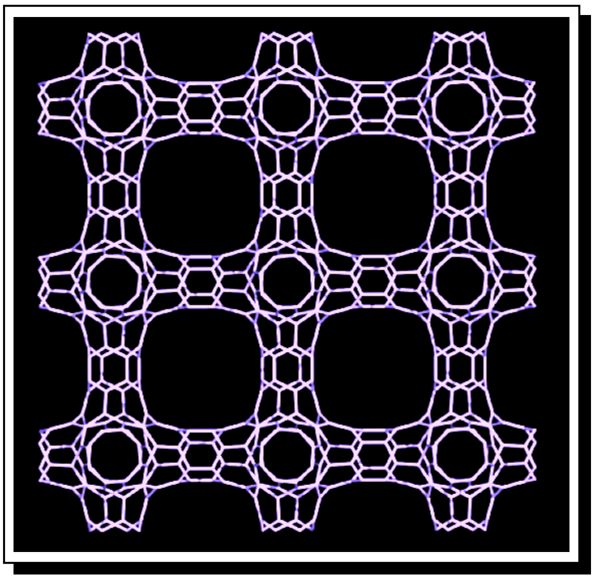

Figure 1. [1–5] A-dimensional lattice of $Cas(C)$-$CaR(C)[m,n,p]$ Nanotubes Junction $\forall\ m,n,p \in \mathbb{N}$.

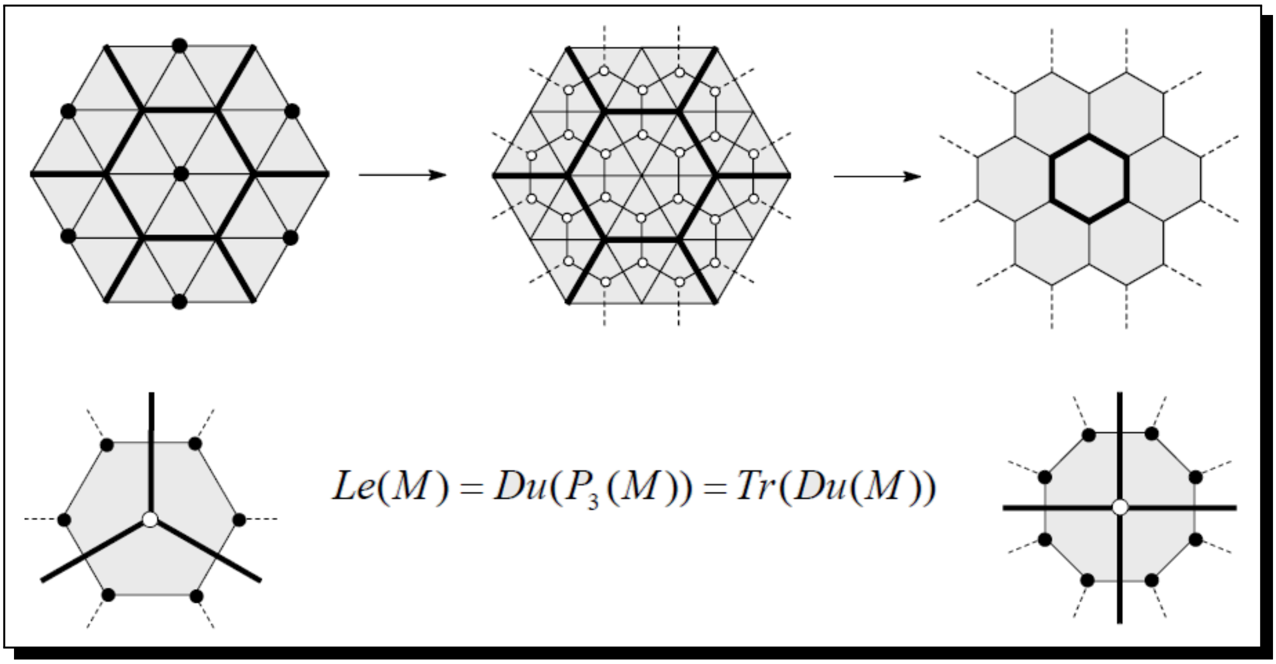

Figure 2. [1–5] An example of "Leapfrog Le(C_6)" graph operation.

Now, consider $Cas(C)$-$CaR(C)[m,n,p]$ Nanotubes Junction $\forall\ m,n,p \in \mathbb{N}$, such that the 3-Dimensional lattice of $Cas(C)$-$CaR(C)[m,n,p]$ Nanotubes Junction are shown in Figure 1. In this paper we name the first member $Cas(C)[1,1,1]$ or $Cas(C)$ as the based unit (see Figure 4), since all member of $Cas(C)[m,n,p]$ Nanotubes are combine this unit.

By Figure 4, we can see that $6 \times 4 = 24$ vertices/atoms of $Cas(C)$ unit have degree 2 (red colored vertices in Figure 3), and there are $2 \times 4 = 8$ vertices/atoms with degree 3 in any split of $Cas(C)$ (yellow colored vertices in Figure 3) and $Cas(C)$ unit has 6 splits. Finally, there are 8 common vertices between 3 joist splits of $Cas(C)$ (obviously with degree 3 and colored by white).

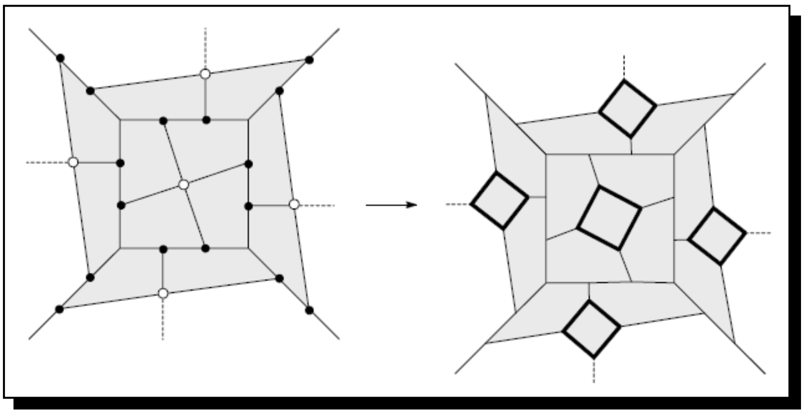

Figure 3. [1–5]An example of "Capra Ca(C_4)" graph operation.

These imply that $Cas(C)$ unit has $24+6\times 8+8=80$ ($|V(Cas(C))|$) vertices/atoms and the number of edges/bonds of $Cas(C)$ unit is equal to

$$|E(Cas(C))|=\frac{2\times|V_2|+3\times|V_3|}{2}=\frac{1}{2}[2\times 24+3\times 56]=216.$$

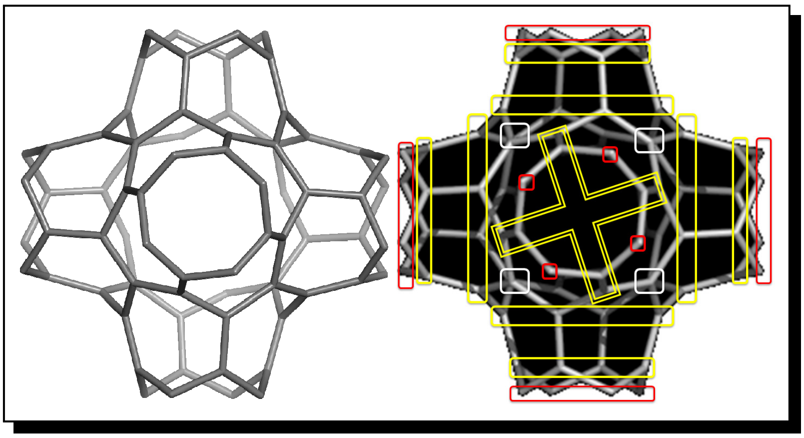

Figure 4. The based unit $Cas(C)$-$CaR(C)[1,1,1]$ of the $Cas(C)$-$CaR(C)[m,n,p]$ Nanotubes Junction $\forall$ $m,n\in\mathbb{N}$.

Thus following M.V. Diudea [5] we denote the number of $Cas(C)$ units in the first rows and column in this Nanotube by integer number m, n and p. Therefore, in general case of this nano-structure $Cas(C)$-$CaR(C)[m,n,p]$, there are $m\times n\times p$ $Cas(C)$ units and there exist $|V(Cas(C)\text{-}CaR(C)[m,n,p])|=80\times m\times n\times p=80mnp$ number of vertices/atoms ($\forall$ $m,n,p\in\mathbb{N}$).

Also, from the structure of $Cas(C)$-$CaR(C)[m,n,p]$ Nanotubes Junction $\forall$ $m,n,p\in\mathbb{N}$, in Figure 4, one can see that the number of edges/bonds of $Cas(C)$-$CaR(C)[m,n,p]$ is equal to

$$\begin{aligned}|E(Cas(C)-CaR(C)[m,n,p])|&=216\times m\times n\times p+4(m-1)(n-1)(p-1)\\&=220mnp-4mn-4mp-4np+4m+4n+4p-4.\end{aligned}$$

Before presenting the main results, let us introduce some definitions.

Definition 1 ([16–18])**.** Let G and d_v $(1 \le d_v \le n-1)$ be a simple connected molecular graph and the vertex degrees of vertices/atom v in G. We divide the vertex set $V(G)$ and edge set $E(G)$ of G into several partitions based on d_v $(\forall\ v \in V(G))$ for $\delta \le k \le \Delta$, $2\delta \le i \le 2\Delta$, and $\delta^2 \le j \le \Delta^2$ as follows

$$V_k = \{v \in V(G) | d_v = k\},$$

$$E_i = \{e = uv \in E(G) | d_u + d_v = i\},$$

$$E_j^* = \{uv \in E(G) | d_u \times d_v = j\},$$

where δ and Δ are the minimum and maximum, respectively, of d_v for all $v \in V(G)$.

In any nanostructure, the degree of an arbitrary vertex/atom of a molecular graph is equal to 1, 2 or 3. Also, the hydrogen atoms in molecular graphs (i.e., vertices of degree 1) are often omitted. Therefore in the case $G = Cas(C)$ unit, we have only

$$V_3 = \{v \in V(Cas(C)) | d_v = 3\},$$

$$V_2 = \{v \in V(Cas(C)) | d_v = 2\}.$$

Because $\forall\ v \in V(Cas(C)d_v = 2$ or 3, and alternatively the edge partitions of $Cas(C)$ are as

$$E_5 = E_6^* = \{uv \in E(Cas(C)) | d_u = 2 \text{ and } d_v = 3\},$$

$$E_6 = E_9^* = \{uv \in E(Cas(C)) | d_u = d_v = 3\}.$$

By according to the Figure 4, its easy to see that the cardinal of these vertex and edge partitions are equal to:

Vertex/Edge partition	V_3	V_2	$E_5 = E_6^*$	$E_6 = E_9^*$
Cardinality	56	24	$2 \times \lvert V_2 \rvert = 48$	168

By these preliminaries, we have main results of this paper in following theorems.

Theorem 1. *Let G be the general case of the nano-structure "$Cas(C)$-$CaR(C)[m,n,p]$ Nanotubes Junction" (see Figure 1). Then,*

- *the atom-bond connectivity index ABC of G is equal to*

$$ABC(Cas(C) - CaR(C)[m,n,p]) = \frac{440}{3}mnp + \left(8\sqrt{2} - \frac{40}{3}\right)(mp + np + mn) + \frac{8}{3}(m + n + p - 1),$$

- *the geometric-arithmetic GA of G is equal to*

$$GA(Cas(C) - CaR(C)[m,n,p]) = 220mnp + \left(\frac{32\sqrt{6}}{5} - 20\right)(mp + np + mn) + 4(m + n + p - 1).$$

Proof. Consider $G = Cas(C) - CaR(C)[m,n,p]$ nano-structure. This nano-structure consists of heptagon and octagon nets (see Figure 1). By above mention results, one can see that the vertex and edge sets of G are equal to $(\forall\ m,n,p \in \mathbb{N})$:

$$|V(Cas(C) - CaR(C)[m,n,p])| = 10(2m)(2n)(2P),$$

$$|E(Cas(C)-CaR(C)[m,n,p])| = 220mnp-4mn-4mp-4np+4m+4n+4p-4.$$

In the general case $G = Cas(C)\text{-}CaR(C)[m,n,p]$ Nanotubes Junction, we can see that $\forall$ $v \in V(Cas(C)\text{-}CaR(C)[m,n,p]) d_v = 2$ or 3, and we have the vertex and edge partitions with their cardinalities as follows ($\forall$ $m,n,p \in \mathbb{N}$).

$V_3 = \{v \in V(G) | d_v = 3\}$,

$V_2 = \{v \in V(G) | d_v = 2\}$.

Vertex partition	V_2	V_3
Cardinality	$4(2mp+2np+2mn)$	$8(10mnp-mp-np-mn)$

$E_5 = E_6^* = \{uv \in E(G) | d_u = 2 \text{ and } d_v = 3\}$,

$E_6 = E_9^* = \{uv \in E(G) | d_u = d_v = 3\}$.

Edge partition	$E_5 = E_6^*$	$E_6 = E_9^*$
Cardinality	$16(mp+np+mn)$	$4(55mnp-5mn-5mp-5np+m+n+p-1)$

Then, we have following computations for the *geometric-arithmetic* (GA) and atom-bond connectivity (*ABC*) indices of $Cas(C)\text{-}CaR(C)[m,n,p]$ Nanotubes Junction ($\forall$ $m,n,p \in \mathbb{N}$).

$$\begin{aligned}
ABC(G) &= \sum_{uv \in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\
&= \sum_{u_1v_1 \in E_9^*} \sqrt{\frac{d_{u_1}+d_{v_1}-2}{d_{u_1} d_{v_1}}} + \sum_{u_2v_2 \in E_6^*} \sqrt{\frac{d_{u_2}+d_{v_2}-2}{d_{u_2} d_{v_2}}} \\
&= \frac{2}{3}|E_9^*| + \frac{\sqrt{2}}{2}|E_6^*| \\
&= \frac{2}{3}(220mnp-20mn-20mp-20np+4m+4n+4p-4) + \frac{\sqrt{2}}{2}(8(2mp+2np+2mn)) \\
&= \frac{8}{3}(55mnp-5mn-5mp-5np+m+n+p-1) + 8\sqrt{2}(mp+np+mn) \\
&= \frac{440}{3}mnp + \left(8\sqrt{2}-\frac{40}{3}\right)(mp+np+mn) + \frac{8}{3}(m+n+p-1)
\end{aligned}$$

and also,

$$\begin{aligned}
GA(G) &= \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \\
&= \sum_{u_1v_1 \in E_9^*} \frac{2\sqrt{d_{u_1} d_{v_1}}}{d_{u_1}+d_{v_1}} + \sum_{u_2v_2 \in E_6^*} \frac{2\sqrt{d_{u_2} d_{v_2}}}{d_{u_2}+d_{v_2}} \\
&= \frac{2\sqrt{9}}{6}|E_9^*| + \frac{2\sqrt{6}}{5}|E_6^*| \\
&= 4(55mnp-5mn-5mp-5np+m+n+p-1) + \frac{2\sqrt{6}}{5}(16(mp+np+mn))
\end{aligned}$$

$$= 220mnp + \left(\frac{32\sqrt{6}}{5} - 20\right)(mp + np + mn) + 4(m + n + p - 1).$$

and this completed the proof. □

3. Conclusion

In this study we have calculated the *geometric-arithmetic* (GA) and atom-bond connectivity (ABC) indices of a special chemical molecular graph "$Cas(C)$-$CaR(C)[m,n,p]$ Nanotubes Junction" are given. The $Cas(C)$-$CaR(C)[m,n,p]$ Nanotubes Junction is a new nano-structure that was defined by M.V. Diudea, on based the new graph operations (Leapfrog Le and Capra Ca) on the cycle graph C_n.

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

References

[1] M.V. Diudea, Nanostructuri Periodice, Operations on Maps, *Periodic Nanostructures* 115-136 (2007).

[2] M.V. Diudea (ed.), *QSPR/QSAR Studies by Molecular Descriptors*, NOVA, New York (2001).

[3] M.V. Diudea, I. Gutman and L. Jäntschi, *Molecular Topology*, NOVA, New York (2002).

[4] M.V. Diudea, M.S. Florescu and P.V. Khadikar, *Molecular Topology and Its Applications*, EFICON, Bucharest (2006).

[5] M.V. Diudea, Phenylenic and naphthylenic tori, *Fullerenes, Nanotubes and Carbon Nanostructures* **10**(4) (2002), 273 – 292.

[6] M.R. Farahani and H. Hosseini, A new method for computing domination polynomials of graphs, *Pacific Journal of Applied Mathematics* 7(3) (2015), 1 – 14.

[7] M.R. Farahani and M.P. Vlad, On the Schultz, Modified Schultz and Hosoya polynomials and derived indices of Capra-designed planar Benzenoids, *Studia Universitatis Babes-Bolyai Chemia.* **4** (2012), 55 – 63.

[8] M.R. Farahani and M.P. Vlad, Computing first and second Zagreb index, first and second Zagreb polynomial of Capra-designed planar benzenoid series Ca_n (C_6), *Studia Universitatis Babes-Bolyai Chemia.* **58**(2) (2013), 133 – 142.

[9] M.R. Farahani and M.P. Vlad, Some connectivity indices of Capra-designed planar Benzenoid series Ca_n (C_6), *Studia Universitatis Babes-Bolyai Chemia.* **60**(2) (2015), 251 – 258.

[10] M.R. Farahani, K. Kato and M.P. Vlad, Second-sum-connectivity index of Capra-designed planar benzenoid series Ca_n (C_6), *Studia Universitatis Babes-Bolyai Chemia.* **58**(2) (2013), 127 – 132.

[11] M.R. Farahani, Second-sum-connectivity index of Capra-designed planar Benzenoid series Can (C6), *Polymers Research Journal* **7**(3) (2013), 1 – 8.

[12] M.R. Farahani, Computing ABC4 index of Capra-designed planar benzenoid series Ca_k (C_6), *Advances in Materials and Corrosion* **1** (2012), 61 – 64.

[13] M.R. Farahani, A new geometric-arithmetic index of a new family of Benzenoid molecular graph, *Chemical Physics Research Journal* **6**(1) (2013), 13 – 19.

[14] M.R. Farahani, The first and second Zagreb polynomials and their corresponding indices of Capra-designed of cycles, *International Journal of Chemical Modeling* **7**(1) (2015), 43 – 52.

[15] M.R. Farahani, On atom bond connectivity and geometric-arithmetic indices of Capra-designed of cycles, *Pacific Journal of Applied Mathematics* **6**(2) (2014), 133 – 141.

[16] M.R. Farahani, Some connectivity indices and Zagreb index of polyhex nanotubes, *Acta Chim. Slov. 59* (2012), 779 – 783.

[17] W. Gao, M. Nazri Husin, M.R. Farahani and M. Imran, On the edges version of atom-bond connectivity index of nanotubes, *J. Comput. Theor. Nanosci.* **13**(10) (2016), 6733 – 6740.

[18] W. Gao, M. Nazri Husin, M.R. Farahani and M. Imran, On the edges version of atom-bond connectivity and geometric arithmetic indices of nanocones $CNCk[n]$, *J. Comput. Theor. Nanosci.* **13**(10) (2016), 6741 – 6746.

[19] W. Gao, M.R. Farahani, Sh. Wang and M. Nazri Husin, On the edge-version atom-bond connectivity and geometric arithmetic indices of certain graph operations, *Applied Mathematics and Computation* **308** (2017), 11 – 17.

[20] Y. Gao, M.R. Farahani and W. Gao, A neighborhood union condition for fractional (k,n',m)-critical deleted graphs, *Transactions on Combinatorics* **6**(1) (2017), 13 – 19.

[21] W. Gao and M.R. Farahani, Degree-based indices computation for special chemical molecular structures using edge dividing method, Applied Mathematics and Nonlinear Sciences **1**(1) (2015), 94 – 117.

[22] M. Randić, On characterization of molecular branching, *J. Amer. Chem. Soc.* **97** (1975), 6609 – 6615.

[23] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley, Weinheim (2000).

[24] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, FL (1992).

[25] D. Vukicevic and B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.* **46** (2009), 1369.

[26] L. Xiao, S. Chen, Z. Guo and Q. Chen, The geometric-arithmetic index of Benzenoid systems and Phenylenes, *Int. J. Contemp. Math. Sciences* **5** (45) (2010), 2225 – 2230.

[27] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947), 7 – 20.