American Journal of Computational and Applied Mathematics 2015, 5(6): 174-177
DOI: 10.5923/j.ajcam.20150506.03

Computing the Atom Bond Connectivity and Geometric-Arithmetic Indices of V-Phenylenic Nanotubes and Nanotori

Mohammad Reza Farahani[1,*], **M. R. Rajesh Kanna**[2]

[1]Department of Applied Mathematics of Iran University of Science and Technology (IUST), Narmak, Tehran, Iran
[2]Post Graduate Department of Mathematics, Maharani's Science College for Women, Mysore, India

Abstract Let G be a simple connected graph and e=uv be an edge bond of G in chemical graph theory. The Geometric-arithmetic GA index is GA(G)= $\sum_{uv\in E(G)}\frac{2\sqrt{d_u d_v}}{d_u+d_v}$ and the Atom-bond connectivity ABC index is defined as ABC(G)= $\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_u d_v}}$ in which degree of a vertex v denoted by dv. In this present study, we compute some results about these connectivity topological indices of V-phenylenic Nanotubes and Nanotori.

Keywords Nanotubes, Molecular graph, Geometric-Arithmetic index, Atom-Bond connectivity index

1. Introduction

Let *G* be a simple connected graph and *e=uv* be an edge of G in graph theory. 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. Also in chemical graph theory, 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".

Chemical graph theory is an important branch of graph theory and Mathematical chemistry, which applies graph theory to mathematical modeling of chemical phenomena [1-6]. A chemical topological index is a numeric quantity from the structural graph of a molecule and is invariant on the automorphism of the graph. One of the important topological connectivity index in chemical graph theory is the *Geometric-Arithmetic index GA* considered by *D. Vukičević* and *B. Furtula* [7] as

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

where d_u and d_v are the degrees of the vertices *u* and *v*, respectively.

Another important connectivity index is the *Atom-Bond Connectivity index ABC* and was introduced by *B. Furtula et al* [8] and is defined as follows:

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

For a comprehensive survey of the mathematical properties and chemical properties of these indices see papers series and books [9-33].

In this paper, we focus on the *Atom-Bond Connectivity index ABC* and the *Geometric-Arithmetic index GA* and compute some results about these connectivity topological indices for two kind of Nano-structures "V-Phenylenic Nanotubes *G=VPHX[m,n]* and V-Phenylenic Nanotorus *H=VPHY[m,n]*".

2. Main Results

The goal of this section is to compute the *Atom-Bond*

* Corresponding author:
MrFarahani88@Gmail.com (Mohammad Reza Farahani)
Mr_Farahani@Mathdep.iust.ac.ir (Mohammad Reza Farahani)
Published online at http://journal.sapub.org/ajcam

Connectivity ABC and the *Geometric-Arithmetic GA* indices of two carbon Nano-structures. The structure of these two carbon Nano-structures "*V-Phenylenic Nanotubes* and *Nanotorus*" are consist of cycles with length four (C_4), six (C_6) and eight (C_8). In other words, in the structure of these nanotubes a $C_4C_6C_8$ net is a trivalent decoration made by alternating C_4, C_6 and C_8. These can cover either a cylinder or a torus. In Figure 1 and Figure 2, a 2-Dimensional lattice of V-Phenylenic Nanotubes $G=VPHX[m,n]$ and V-Phenylenic Nanotorus $H=VPHY[m,n]$ are shown ($\forall m,n>1$).

Let we denote the number of hexagon in the first row of the 2D-lattice of *V-Phenylenic* G and H by m and alternatively we denote the number of hexagon in the first column by n. From Figures 1 and 2, we see that in each period, there are *6* vertices and we have mn repetition. Thus the number of vertices in *V-Phenylenic* G and H is equal to $|V(VPHX[m,n])|=|V(VPHY[m,n])|=6mn$. Since there are m vertices with degree two in the first row and m vertices with degree two in the last row, too and other vertices have degree three, then the number of edges in V-Phenylenic Nanotubes $G=VPHX[m,n]$ ($\forall m,n>1$) is equal to

$$|E(VPHX[m,n])|=\frac{2(2m)+3(6mn-2m)}{2}=9mn-m$$

On other hands, since all vertices in V-Phenylenic Nanotorus $H=VPHY[m,n]$ ($\forall m,n>1$), have degree three, thus,

$$|E(VPHY[m,n])|=\tfrac{1}{2}\times 3(6mn)=9mn.$$

For a review, historical details and further bibliography see references [33-42]. Now we compute the ABC and GA indices of the V-Phenylenic Nanotubes and V-Phenylenic Nanotorus by $G=VPHX[m,n]$ and $H=VPHY[m,n]$ ($\forall m, n\in\mathbb{N}-\{1\}$),

Theorem 1. Let G be the V-Phenylenic Nanotubes $VPHX[m,n]$ and H be the V-Phenylenic Nanotorus $VPHY[m,n]$ for every $m,n\in\mathbb{N}-\{1\}$, then

- Geometric-Arithmetic index of G is equal to

$$GA(VPHX[m,n])=(9mn-5m)+\frac{8\sqrt{6}}{5}m$$

- Atom-Bond Connectivity index of G is equal to

$$ABC(VPHX[m,n])=(3n+\frac{4\sqrt{3}-10}{3})m$$

- Geometric-Arithmetic index of H is equal to

$GA(H)=|E(VPHY[m,n])|=9mn$

- Atom-Bond Connectivity index of H is equal to

$ABC(H)=|V(VPHY[m,n])|=6mn$

Before prove the main results in Theorem 1, let us introduce following definition.

Definition 1. [32] For a connected graph $G=(V(G),E(G))$ with the minimum and maximum of degrees $\delta=Min\{d_v|v\in V(G)\}$ and $\Delta=Max\{d_v|v\in V(G)\}$, respectively, there exist vertex.atom and edge/bond partitions as follow

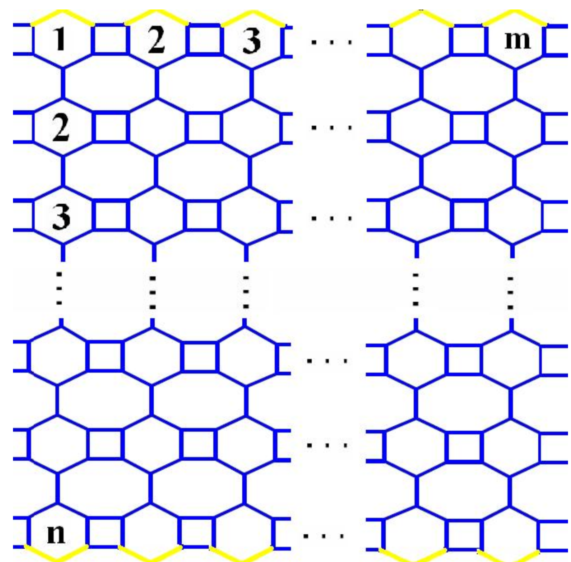
$\forall k$: $\delta\le k\le\Delta$, $V_k=\{v\in V(G)|\ d_v=k\}$

$\forall i$: $2\delta\le i\le 2\Delta$, $E_i=\{e=uv\in E(G)|d_u+d_v=i\}$

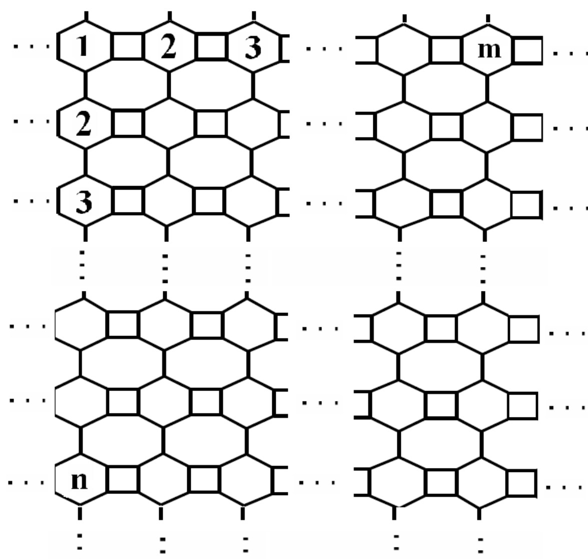
$\forall j$: $\delta^2\le j\le\Delta^2$, $E_j{}^*=\{uv\in E(G)|d_u\times d_v=j\}$.

Thus, the edge set of V-Phenylenic Nanotubes $G=VPHX[m,n]$ can be dividing to two partitions, e.g. E_5 and E_6, as follow:

- For every $e=uv$ belong to E_6, $d_u=d_v=3$ or
  $E_5=E_6{}^*=\{uv\in E(VPHX[m,n])|d_u+d_v=5\ \&\ d_u\times d_v=6\}$
- For every $e=uv$ belong to E_5, then $d_u=2$ and $d_v=3$ or
  $E_6=E_9{}^*=\{uv\in E(VPHX[m,n])|d_u+d_v=6\ \&\ d_u\times d_v=9\}$.



G=VPHX[m,n]



H=VPHY[m,n]

Figure 1. The 2-Dimensional lattice of V-Phenylenic Nanotubes $G=VPHX[m,n]$ and V-Phenylenic Nanotorus $H=VPHY[m,n]$

Also, all member in edge set of V-Phenylenic Nanotorus *VPHY[m,n]* exist in a following partition E_6 or E_9* since all vertices/atoms have degree three.

$$E_6=E_9^*=\{uv\in E(VPHY[m,n])|d_u+d_v=6\ \&\ d_u\times d_v=9\}$$
$$=E(VPHY[m,n])$$

Proof. Consider V-Phenylenic Nanotubes *G=VPHX[m,n]* with *6mn* vertices and 9*mn-m* edges. By according to the 2-Dimensional lattice of *G=VPHX[m,n]* in Figure1, we mark all edges from E_5 or E_6* by yellow color and all member from E_6 or E_9* by blue color then we see that in V-Phenylenic Nanotubes *G=VPHX[m,n]* $|E_5|=|E_6^*|$ = *2m+2m* and also $|E_6|=|E_9^*|=9mn-5m$.

Now, we have following computations for the *Atom-Bond Connectivity index ABC* and the *Geometric-Arithmetic index GA* of V-Phenylenic Nanotubes *VPHX[m,n]* as follow:

$$ABC(VPHX[m,n])=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$$

$$=\sum_{e=uv\in E_9^*}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}+\sum_{e=uv\in E_6^*}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$$

$$=|E_6|\sqrt{\frac{6-2}{9}}+|E_5|\sqrt{\frac{5-2}{6}}$$

$$=(9mn-5m)\ \frac{2}{3}+4\frac{\sqrt{3}}{3}\ m$$

$$=(3n+\frac{4\sqrt{3}-10}{3})m$$

$$GA(VPHX[m,n])=\sum_{uv\in E(VPHX[m,n])}\frac{2\sqrt{d_ud_v}}{d_u+d_v}$$

$$=\sum_{e=uv\in E_9^*}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{e=uv\in E_6^*}\frac{2\sqrt{d_ud_v}}{d_u+d_v}$$

$$=|E_9^*|\frac{2\sqrt{9}}{6}+|E_6^*|\frac{2\sqrt{6}}{5}$$

$$=(9mn-5m)+\frac{8\sqrt{6}}{5}m$$

Finally, Consider V-Phenylenic Nanotorus *H=VPHY[m,n]* with *6mn* vertices and 9*mn* edges. And by according to the 2-Dimensional lattice of *H* in Figure1, we see that all member of single edge partition E_6 (or E_9*) are mwrked by black color, such that in *H=VPHY[m,n]* $(\forall m,n\in\mathbb{N}-\{1\})$, $|E_6|=|E_9^*|=9mn=|E(VPHY[m,n])|$. Therefore the *Atom-Bond Connectivity index ABC* and the *Geometric-Arithmetic index GA* of V-Phenylenic Nanotorus *H=VPHY[m,n]* are equal to:

$$ABC(VPHY[m,n])=\sum_{uv\in E(H)}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$$

$$=|E_9^*|\sqrt{\frac{6-2}{9}}$$

$$=(9mn)\ \frac{2}{3}=6mn=|V(VPHY[m,n])|$$

$$GA(VPHY[m,n])=\sum_{uv\in E(H)}\frac{2\sqrt{d_ud_v}}{d_u+d_v}$$

$$=|E_9^*|\frac{2\sqrt{9}}{6}$$

$$=(9mn)\ \frac{2\times 6}{6}=9mn=|E(VPHY[m,n])|$$

And these completed the proof of theorem.

ACKNOWLEDGEMENTS

Authors are also thankful to the University Grants Commission, Government of India, for the financial support under the Grant MRP(S)-0535/13-14/KAMY004/ UGC-SWRO.

REFERENCES

[1] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* 69(1947), 17-20.

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

[3] L.B. Kier, L. H. Hall, Molecular Connectivity in Structure-Activity Analysis. *Research Studies Press/Wiley, Letchworth/New York*, (1986).

[4] M. Randić, On characterization of molecular branching. *J. Am. Chem. Soc.* 97 (1975), 6609-6615.

[5] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.

[6] N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton, FL, 1992.

[7] D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. *J. Math. Chem.* 46(2009), 1369-1376.

[8] B. Furtula, A. Graovac, D. Vukičević, Disc. Appl. Math., 157, 2828 (2009).

[9] Y. Yuan, B. Zhou, N. Trinajstić, On geometric-arithmetic index, *J. Math. Chem.* 47(2010), 833-841.

[10] A. R. Ashrafi and H. Shabani, GA index and Zagreb indices of nanocones, Optoelectron. Adv. Mater.–Rapid Commun., 4(11), 1874-1876 (2010).

[11] M. Ghorbani, GA index of $TUC_4C_8(R)$ nanotube, Optoelectron. Adv. Mater.–Rapid Commun., 4(2), 261-263 (2010).

[12] A. Iranmanesh and M. Zeraatkar, Computing GA index for some nanotubes, Optoelectron. Adv. Mater.–Rapid Commun., 4(11), 1852-1855 (2010).

[13] A. Khaksar, M. Ghorbani, H. R. Maimani, On atom bond connectivity and GA indices of nanocones, Optoelectron. Adv. Mater.–Rapid Commun., 4(11), 1868-1870 (2010).

[14] H. Shabani and A. R. Ashrafi, Computing the GA index of nanotubes and nanotori, Optoelectron. Adv. Mater.–Rapid Commun., 4(11), 1860-1862 (2010).

[15] 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.

[16] M. Zaeembashi and M. Ghorbani, Computation of two classes of GA index of some nanostructures, Optoelectron. Adv. Mater.–Rapid Commun., 4(9), 1415-1418 (2010).

[17] A. Iranmanesh, M. Zeraatkar. Computing Ga index for some nanotubes. Optoelectron. Adv. Mater.–Rapid Commun., 4(11), 1852 - 1855 (2010).

[18] M.R. Farahani. Computing Randic, Geometric-Arithmetic and Atom-Bond Connectivity indices of Circumcoronene Series of Benzenoid. Int. J. Chem Model(Nova). 5(4), (2013), 485-493.

[19] M.R. Farahani. Computing Randic, Geometric-Arithmetic and Atom-Bond Connectivity indices of Circumcoronene Series of Benzenoid. Int. J. Chem Model(Nova). 5(4), (2013), 485-493.

[20] M.R. Farahani. Computing some connectivity indices of Nanotubes. Adv. Mater. Corrosion 1 (2012) 57-60.

[21] M.R. Farahani. Some Connectivity index of an infinite class of Dendrimer Nanostars. Journal of Applied Physical Science International(IK press), 2015, 3(3), 99-105.

[22] M.R. Farahani, M.P. Vlad. Some Connectivity Indices of Capra-Designed Planar Benzenoid Series $Ca_n(C_6)$. Studia Universitatis Babes-Bolyai Chemia. (2015), In press.

[23] M.R. Farahani. Computing a New Version of Atom-Bond Connectivity Index of Circumcoronene Series of Benzenoid H_k by Using Cut Method Journal of Mathematical Nanoscience. 2(1), (2012), 15-20.

[24] M.R. Farahani. A Version of Atom-Bond Connectivity Index of Circumcoronene Series of Benzenoid. Pacific Journal of Applied Mathematics. 5(4), 245-252, (2013).

[25] M.R. Farahani. Computing a New Connectivity Index for a Famous Molecular Graph of Benzenoid Family. Journal of Chemica Acta 2 (2013) 26-31.

[26] M.R. Farahani. On The Geometric-Arithmetic And Atom Bond Connectivity Index Of $HAC_5C_6C_7[p,q]$ Nanotube. Chemical Physics Research Journal. 6(1), (2013), 21-26.

[27] M.R. Farahani. Atom Bond Connectivity And Geometric-Arithmetic Indices Of $HAC_5C_7[p,q]$ Nanotube. Int. J. Chemical Modeling. 5(1), 127-132, (2013).

[28] M.R. Farahani. New Version of Atom-Bond Connectivity Index of TURC4C8(S). Int J Chem Model. 4(4), 527-531, (2012).

[29] M.R. Farahani. Connectivity Indices of Pent-Heptagonal Nanotubes VAC5C7[p,q]. Advances in Materials and Corrosion. 2, (2013), 33-35.

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

[31] M.R. Farahani. On Atom Bond Connectivity and Geometric-Arithmetic indices of a Benzenoid System. Int. J. Engineering and Technology Research. 3(2), March 2015, 1-4.

[32] M.R. Farahani. Some Connectivity Indices and Zagreb Index of Polyhex Nanotubes. Acta Chim. Slov. 59, 779–783 (2012).

[33] M. Ghorbani, H. Mesgarani and S. Shakeraneh, Computing *GA* index and *ABC* index of V–phenylenic nanotube, Optoelectron. Adv. Mater.–Rapid Commun., 5(3), 324-326 (2011).

[34] M.V. Diudea, *Fuller. Nanotub. Carbon Nanostruct,* 10, 273 (2002).

[35] V. Alamian, A. Bahrami and B. Edalatzadeh, *PI* Polynomial of V-Phenylenic Nanotubes and Nanotori. *Int. J. Mol. Sci.* (2008), *9*, 229-234.

[36] J. Asadpour, Some topological polynomial indices of nanostructures, *Optoelectron. Adv. Mater.–Rapid Commun.* 2011, *5(7),* 769–772.

[37] A. Bahrami and J. Yazdani, Vertex PI Index of V-Phenylenic Nanotubes and Nanotori. *Digest Journal of Nanomaterials and Biostructures,* 2009, *4(1*), 141 - 144.

[38] M. DavoudiMonfared, A. Bahrami and J. Yazdani, PI Polynomial of V-Phenylenic Nanotubes. *Digest Journal of Nanomaterials and Biostructures,* 2010, *5(2),* 441–445.

[39] N. PrabhakaraRao and K.L. Lakshmi. Eccentricity Connectivity Index of V-Phenylenic Nanotubes. *Digest Journal of Nanomaterials and Biostructures,* 2010, *6(1),* 81-87.

[40] M.R. Farahani. Computing GA_5 index of V-Phenylenic Nanotubes and Nanotori. Int. J. Chem Model (Nova).5(4), (2013), 479-484.

[41] M.R. Farahani. Computing fourth atom-bond connectivity index of V-Phenylenic Nanotubes and Nanotori. Acta Chimica Slovenica. 60(2), (2013), 429–432.

[42] M.R. Farahani. Computing Theta Polynomial and Theta Index of V-phenylenic Planar, Nanotubes and Nanotoris. International Journal of Theoretical Chemistry. 1(1), (2013), 01-09.