Acta Universitatis Apulensis
ISSN: 1582-5329

No. 36/2013
pp. 277-284

THE EDGE VERSION OF ATOM-BOND CONNECTIVITY INDEX OF CONNECTED GRAPH

M. Reza Farahani

Abstract. The atom-bond connectivity index is a topological index was 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 d_v. Now we define a new version of ABC index as $ABC_e(G) = \sum_{ef\in E(L(G))} \sqrt{\frac{d_e+d_f-2}{d_e d_f}}$, where d_e denotes the degree of an edge e in G. The goal of this paper is to further the study of the ABC_e index of graphs.

2000 *Mathematics Subject Classification*: 65Lxx, 65L05.

1. Introduction

A graph is a collection of points and lines connecting them. The points and lines of a graph are also called vertices and edges respectively. If e is an edge of G, connecting the vertices u and v, then we write $e = uv$ and say "u and v are adjacent". A connected graph is a graph such that there is a path between all pairs of vertices. The distance $d(u, v)$ between two vertices u and v is the length of the shortest path between u and v in G. A simple graph is an unweighted, undirected graph without loops or multiple edges. A single number that can be used to characterize some property of the graph is called a *Topological Index* for that graph. Obviously, the number of vertices and the number of edges are topological indices. The *Wiener index* is the first graph invariant reported (distance based) topological index and is defined as a half sum of the distances between all the pairs of vertices in a graph [1]. Also, the edge version of Wiener index which were based on distance between edges introduced by *A. Iranmanesh et al.* in 2008 [2]. These topological indices are formulated as follow:

$$W_v(G) = \sum_{\{u,v\}\subset V(G)} d(u, v) \quad (1)$$

$$W_e(G) = \sum_{\{e,f\}\subset E(G)} d(e, f) \quad (2)$$

in which degree of vertex v and edge e denoted by d_v and d_e.

The degree of a vertex v is the number of vertices joining to v. Also, the degree of an edge $e \in E(G)$ is the number of its adjacent vertices in $V(L(G))$, where the line graph $L(G)$ of a graph G is defined to be the graph whose vertices are the edges of G, with two vertices being adjacent if the corresponding edges share a vertex in G.

A class of atom-bond connectivity indices may be defined as

$$ABC_{general}(G) = \sum_{uv \in E(G)} \sqrt{\frac{Q_u + Q_v - 2}{Q_u \times Q_v}} \tag{3}$$

where Q_v is some quantity that in a unique manner can be associated with the vertex v of the graph G. The first member of this class was considered by *E. Estrada et. al.* [3], by setting Q_v and Q_u to be the degree of a vertex v and u:

$$ABC_1(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \times d_v}} \tag{4}$$

The second member of this class was considered by *A. Graovac* and *M. Ghorbani* [4] in 2010 by setting Q_u to be the number n_u of vertices of G lying closer to the vertex u than to the vertex v for the edge uv of the graph G ($n_u = \{y | y \in V(G), d(u,y) < d(y,v)\}$):

$$ABC_2(G) = \sum_{uv \in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u \times n_v}} \tag{5}$$

The third member of this class was considered by *M.R. Farahani* [5]

$$ABC_3(G) = \sum_{uv \in E(G)} \sqrt{\frac{m_u + m_v - 2}{m_u \times m_v}} \tag{6}$$

where m_u denotes the number of vertices of G whose distances to vertex u are smaller than those to other vertex v of the edge $e = uv$ and m_v is defined analogously. The fourth member of this class was considered by *M. Ghorbani et al.* [6] as:

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u \times S_v}} \tag{7}$$

in which $S_u = \sum_{v \in N_G(u)} d_v$ and $N_G(u) = \{v \in V(G) | uv \in E(G)\}$. The fifth member of this class was introduced by *M.R. Farahani* [7] by setting Q_u to be the number ϵ_u the eccentricity of vertex u:

$$ABC_5(G) = \sum_{uv \in E(G)} \sqrt{\frac{\epsilon_u + \epsilon_v - 2}{\epsilon_u \times \epsilon_v}} \tag{8}$$

Here, we define the new member (*edge version of atom-bond connectivity index*) of this class on the ground of the end-vertex degree d_e and d_f of edges e and f in a line graph of G as follows:

$$ABC_e(G) = \sum_{ef \in E(L(G))} \sqrt{\frac{d_e + d_f - 2}{d_e \times d_f}} \tag{9}$$

where d_e denotes the degree of the edge e in G. The reader can find more information about the atom-bond connectivity index in [8-16]. The goal of this paper is to further the study of the ABC_e index.

2. Main Result

The goal of this section is to study and computing the ABC_e index of the complete graph K_n, path P_n, cycle C_n and star graph S_n. In continue we obtain a closed formula of this index for a famous molecular graph that is *Circumcoronene Series of Benzenoid* H_k. For every positive integer number k, the general form of circumcoronene series of benzenoid H_k is shown in Figure 1. Also, its line graph is shown in Figure 2. For more information of this family, see the paper series [7, 10, 16-23].

Lemma 1. *Let K_n be the complete graph on n vertices. Then $L(K_n)$ will be a $(2n-2)$_regilar graph and for every $e \in E(K_n)$ (or $e \in V(L(K_n))$) $d_v = 2(n-1)$. So $|E(L(K_n))| = \frac{1}{2}|E(K_n)|2(n-1) = \frac{1}{2}n(n-1)^2$. This implies that*

$$ABC_e(K_n) = \sum_{ef \in E(L(K_n))} \sqrt{\frac{d_e + d_f - 2}{d_e d_f}} =$$

$$|E(L(K_n))| \sqrt{\frac{2(n-1) + 2(n-1) - 2}{2(n-1) \times 2(n-1)}} = \frac{n(n-1)\sqrt{4n-6}}{4} \tag{10}$$

Lemma 2. *Let C_n be the cycle of length n. Then one can see that $L(C_n) = C_n$ and for every $v \in V(C_n)$ and $e \in V(L(C_n))$ $d_v = d_e = 2$, So*

$$ABC_e(C_n) = |E(L(C_n))| \sqrt{\frac{2+2-2}{2 \times 2}} = \frac{\sqrt{2}}{2} n \tag{11}$$

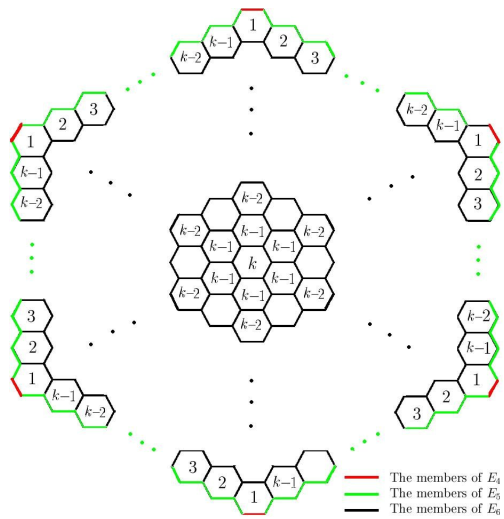

Figure 1: The Circumcoronene Series of Benzenoid $H_k (k \geq 1)$ with edges marking. [16]

Lemma 3. *Let P_n be a path of length n. Then $L(P_n) = P_{n-1}$ and for all vertices of $L(P_n)$: $de = 2$, (except first and end vertices on path, that are as degree one), thus*

$$ABC_e(P_n) = (n-3)\sqrt{\frac{2+2-2}{2\times 2}} + (2)\sqrt{\frac{1+2-2}{1\times 2}} = \frac{\sqrt{2}}{2}(n-1) \quad (12)$$

Lemma 4. *Let S_n be a star graph with $n+1$ vertices. Then $L(S_n)$ will be a $(n-1)$_regilar graph (or a complete graph on n vertices) and for every $e \in E(S_n)$ (or $e \in V(L(S_n))$) $d_v = n-1$. So $|E(L(S_n))| = |E(K_n)| = \frac{1}{2}n(n-1)$. This implies that*

$$ABC_e(S_n) = |E(L(S_n))|\sqrt{\frac{(n-1)+(n-1)-2}{(n-1)\times(n-1)}} = \frac{n\sqrt{2n-4}}{2} = ABC_1(K_n) \quad (13)$$

Theorem 5. *Let G be the graphs from the circumcoronene series of benzenoid H_k $\forall k \geq 1$ with $6k^2$ vertices and $9k^2 - 3k$ edges, then*

$$ABC_1(H_k) = 6k^2 + (6\sqrt{2} - 10)k + (4 - 3\sqrt{2}) \quad (14)$$

$$ABC_e(H_k) = \frac{9}{2}\sqrt{6}k^2 + \left(8 + 2\sqrt{15} - 9\sqrt{6}\right)k + \left(\frac{9}{2}\sqrt{6} - 2\sqrt{15} + 6\sqrt{2} - 12\right) \quad (15)$$

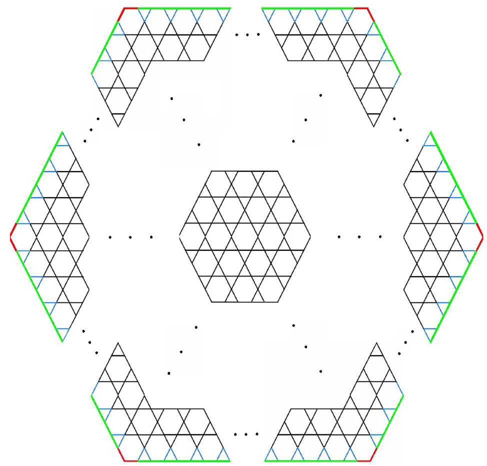

Figure 2: The general representation of line graph of Circumcoronene Series of Benzenoid $H_k (k \geq 1)$ with edges marking. [19]

Proof. Consider the circumcoronene series of benzenoid H_k, for all positive integer number k. The first part of theorem proved in ref. [16]. So we start the proof of second part, immediately. By refer to Proposition 1, the edge version of atom-bond connectivity index of H_k is equivalent with atom-bond connectivity index of its line graph. At first, we category the vertex set and edge set of H_k as follow:

$V_3 = \{v \in V(H_k) | d_v = 3\} \Rightarrow |V_3| = 6k(k-1)$
$V_2 = \{v \in V(H_k) | d_v = 2\} \Rightarrow |V_2| = 6k$
$E_4 = \{e = uv \in E(H_k) | d_u = d_v = 2\} \Rightarrow |E_4| = 6$
$E_5 = \{e = uv \in E(H_k) | d_u = 3 \& d_v = 2\} \Rightarrow |E_5| = 12(k-1)$
$E_6 = \{e = uv \in E(H_k) | d_u = d_v = 3\} \Rightarrow |E_6| = 9k^2 - 15k + 6$

In Figure 1, all edges belong to E_4, E_5 and E_6 marked by red, green and black colors, respectively. It is easy to see that $\forall k \geq 1$; $L(H_k)$ has $9k^2 - 3k$ vertices and from $\frac{4(9k^2-15k+6)+3\times12(k-1)+2\times6}{2} = 18k^2 - 12k$ edges. Alternatively, we can category the vertex set and edge set of $L(H_k)$ by using the results of ref.[19] as follow:

$VL_2 = \{e \in E(H_k) | d_e = 2\} \Rightarrow |VL_2| = |E_4| = 6$
$VL_3 = \{e \in E(H_k) | d_e = 3\} \Rightarrow |VL_3| = |E_5| = 12(k-1)$
$VL_4 = \{e \in V(L(H_k)) \ or \ e \in E(H_k) | d_e = 4\} \Rightarrow |VL_4| = |E_6| = 9k^2 - 15k + 6$

$EL_5 = \{\mu = ef \in E(L(H_k)) | d_e = 2, d_f = 3\} \Rightarrow |EL_5| = 2|VL_2| = 12$

$EL_6 = \{\mu = ef \in E(L(H_k)) | d_e = \quad d_f = 3\} \Rightarrow |EL_6| = |VL_3| - |VL_2| = 6(2k-3)$
$EL_7 = \{\mu = ef \in E(L(H_k)) | d_e = 3, d_f = 3\} \Rightarrow |EL_7| = |VL_3| - |VL_2| = 12(k-1)$
$EL_8 = \{\mu = ef \in E(L(H_k)) | d_e = d_f = 4\} \Rightarrow |EL_8| = |E(L(H_k))| - |EL_7| - |EL_6| - |EL_5|$
$\Rightarrow \qquad = 18k^2 - 36k + 18 = 18(k-1)^2.$

Similar above, in Figure 2 all edges belong to EL_5, EL_6, EL_7 and EL_8 marked by red, green and black colors, respectively.

$$\begin{aligned}
ABC_e(H_k) &= \sum_{ef \in E(L(H_k))} \sqrt{\frac{d_e + d_f - 2}{d_e d_f}} \\
&= \sum_{ef \in EL_5} \sqrt{\frac{3+2-2}{3 \times 2}} + \sum_{ef \in EL_6} \sqrt{\frac{3+3-2}{3 \times 3}} + \sum_{ef \in EL_7} \sqrt{\frac{4+3-2}{4 \times 3}} + \sum_{ef \in EL_8} \sqrt{\frac{4+4-2}{4 \times 4}} \\
&= \frac{\sqrt{2}}{2}|EL_5| + \frac{2}{3}|EL_6| + \frac{\sqrt{15}}{6}|EL_7| + \frac{\sqrt{6}}{4}|EL_8| \\
&= \frac{\sqrt{2}}{2}(12) + \frac{2}{3}(12k-18) + \frac{\sqrt{15}}{6}(12k-12) + \frac{\sqrt{6}}{4}(18k^2 - 36k + 18) \\
&= \frac{9}{2}\sqrt{6}k^2 + \left(8 + 2\sqrt{15} - 9\sqrt{6}\right)k + \left(\frac{9}{2}\sqrt{6} - 2\sqrt{15} + 6\sqrt{2} - 12\right) \qquad (16)
\end{aligned}$$

And it completes the proof.

Example 1. *Let H_3 be the Circumcoronene. Then the number of edges e_5, e_6, e_7 and e_8 in line graph H_3 are equal to 12, 18, 24 and 72, respectively (see Figure 3). So ABC_e index of H_3 is equal to $ABC_e(H_3) = ABC(L(H_3)) = 80.0681$.*

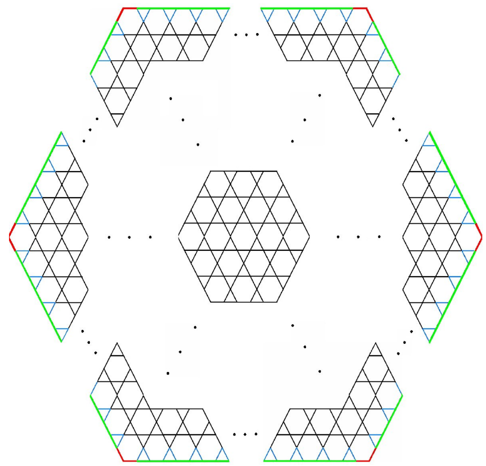

Figure 3: The representation of Circumcoronene H_3 and its line graph $(L(H_3))$. [19]

References

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

[2] A. Iranmanesh, I. Gutman, O. Khormali, A. Mahmiani, MATCH Commun. Math. Comput. Chem. 61(3), (2009), 663.

[3] E. Estrada, L. Torres, L. Rodriguez, I. Gutman, Indian J. Chem. 1998, 37A, 849-855.

[4] A. Graovac, M. Ghorbani, *A New Version of Atom-Bond Connectivity Index*, Acta Chim. Slov. 57, 609-612, (2010).

[5] M.R. Farahani, *A New Version of Atom-Bond Connectivity Index of Circumcoronene Series of Benzenoid*, Submitted for publication (2013).

[6] M. Ghorbani, M.A. Hosseinzadeh *Computing ABC_4 index of nanostar dendrimers*, Optoelectron. Adv. Mater.-Rapid Commun. 4(9), (2010), 1419 - 1422.

[7] M.R. Farahani, *Eccentricity Version of Atom-Bond Connectivity Index of Benzenoid Family $ABC5(H_k)$*, World Applied Sciences Journal, (2013), 21(9), 1260-1265.

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

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

[10] M.R. Farahani *A New Version of Atom-Bond Connectivity Index of Circumcoronene Series of Benzenoid*, J. Math. Nano Science. 2(1), (2012), 15-20.

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

[12] A. Madanshekaf, M. Ghaneeei, *Computing two topological indices of nanostars dendrimer*, Optoelectron. Adv. Mater.-Rapid Commun. 4(12), (2010), 2200-2202.

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

[14] M. B. Ahmadi, M. Saseghimehr, *Atom bond connectivity index of an infinite class $NS_1[n]$ of dendrimer nanostars*, Optoelectron. Adv. Mater.-Rapid Commun. 4(7), (2010), 1040-1042.

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

[16] M.R. Farahani, *Computing Randic, Geometric-Arithmetic and Atom-Bond Connectivity indices of Circumcoronene Series of Benzenoid*, Int. J. Chem. Model. 5(5), (2013), In press.

[17] V. Chepoi S. Klavzar, *Distances in benzenoid systems: Further developments*, Discrete Math. 192, (1998) 27-39.

[18] M.V. Diudea, Studia Univ. Babes-Bolyai, 4, (2003) 3-21.

[19] M.R. Farahani, *The Edge Version of Geometric-Arithmetic Index of Benzenoid Graph*, Romanian Academy Seri B. 15(2). (2013). In press.

[20] S. Klavzar, I. Gutman, B. Mohar, *Labeling of Benzenoid Systems which Reflects the Vertex-Distance Relations*, J. Chem. Int Comput. Sci. 35, (1995) 590-593.

[21] S. Klavzar, *A Bird's Eye View of The Cut Method And A Survey of Its Applications In Chemical Graph Theory*, MATCH Commun. Math. Comput. Chem. 60, (2008), 255-274.

[22] A. Soncini, E. Steiner, P.W. Fowler, R.W.A. Havenith, L.W. Jenneskens. *Perimeter Effects on Ring Currents in Polycyclic Aromatic Hydrocarbons: Circumcoronene and Two Hexabenzocoronenes*, Chem. Eur. J. 9, (2003) 2974-2981.

[23] P. Zigert, S. Klavzar, I. Gutman. *Calculating the hyper-Wiener index of benzenoid hydrocarbons*, ACH Models Chem. 137, (2000) 83-94.

Mohammad Reza Farahani
Department of Mathematics
Iran University of Science and Technology
(IUST) Narmak, Tehran 16844, Iran
email: *Mr_Farahani@mathdep.iust.ac.ir, MrFarahani88@gmail.com*