STUDIA UBB CHEMIA, LX, 2, Tom II, 2015 (p. 251-258)
(RECOMMENDED CITATION)

SOME CONNECTIVITY INDICES OF CAPRA-DESIGNED PLANAR BENZENOID SERIES $Ca_n(C_6)$

MOHAMMAD REZA FARAHANI[a], MIRANDA PETRONELLA VLAD[b]

ABSTRACT. A molecular graph can be transformed using map operations, one of these, named Capra, being defined by *Diudea*. In this paper, we focus on the structure of *Capra-designed planar benzenoid series* $Ca_n(C_6)$ ($k≥0$) and compute some connectivity indices of this family. A connectivity index is a real number related to a molecular graph and is invariant under graph automorphism.

Keywords: *Benzenoid, Capra map operation, Connectivity index.*

INTRODUCTION

Let $G=(V,E)$ be a molecular graph with the vertex set $V(G)$ and the edge set $E(G)$. $|V(G)|=n$, $|E(G)|=e$ are the number of vertices and edges. In chemical graph theory, the vertices and edges correspond to the atoms and bonds, respectively; the number of incident edges in the vertex v is its degree, denoted by d_v. The vertices u and v are adjacent if there exist an edge $e=uv$ between them. A molecular graph is a connected graph, i.e. there exist a path between any pair of vertices.

A variety of topological indices have been defined; a topological index is a real number related to the structure of graph, which is invariant under graph automorphism.

In 1975 Randić proposed a structural descriptor called the branching index [1-4] that later named the Randić molecular connectivity index (or simply Randić index). It is defined as:

$$\chi(G)=\sum_{e=uv\in E(G)}\frac{1}{\sqrt{d_u d_v}}$$

[a] *Department of Mathematics of Iran University of Science and Technology, (IUST) Narmak, Tehran 16844, Iran, Mr_Farahani@Mathdep.iust.ac.ir*
[b] *Dimitrie Cantemir University, Bucharest, Faculty of Economic Sciences, No 56 Teodor Mihali Street, 400591, Cluj Napoca, Romania, mirandapv@yahoo.com*

Recently, a version, called the Sum-connectivity index, was introduced by *Zhou* and *Trinajstić* [5,6]:

$$X(G)=\sum_{v_u v_v}\frac{1}{\sqrt{d_u+d_v}}$$

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

More recently, *Vukicevic* and *Furtula* [7] proposed two topological indices, named *geometric-arithmetic index* and *atom-bond connectivity index* (denoted by *GA(G)* and *ABC(G),* respectively), see [7-9]. They are defined as follows:

$$GA(G)=\sum_{e=uv\in E(G)}\frac{2\times\sqrt{d(u)d(v)}}{d(u)+d(v)}$$

$$ABC(G)=\sum_{e=uv\in E(G)}\sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$$

Definition 1. Let *G* be a molecular graph and d_v being the degree of vertex $v\in V(G)$. We divide the vertex set *V(G)* and edge set *E(G)* of *G* into several partitions, as follow:

$$\forall i,\delta<i<\Delta, V_i=\{v\in V(G)\,|\,d_v=i\},$$
$$\forall j,2\delta\le j\le 2\Delta, E_j=\{e=uv\in E(G)\,|\,d_v+d_u=j\}$$
$$\forall k,\delta^2\le k\le \Delta^2, E_k^*=\{e=uv\in E(G)\,|\,d_v\times d_u=k\}.$$

Note that $\delta=Min\{d_v\,|v\in V(G)\}$ and $\Delta=Max\{d_v\,|v\in V(G)\}$.

MAIN RESULTS AND DISCUSSION

In this section, we compute Randić connectivity index, sum- connectivity index, geometric-arithmetic index and atom-bond connectivity index of Capra-designed planar benzenoid series $Ca_k(C_6)$.

A mapping is a new drawing of an arbitrary planar graph *G* on the plane. Capra map operation was introduced by *Diudea* [10,11]. This method enables one to build a new structure, according to Figure 1 and Definition 2:

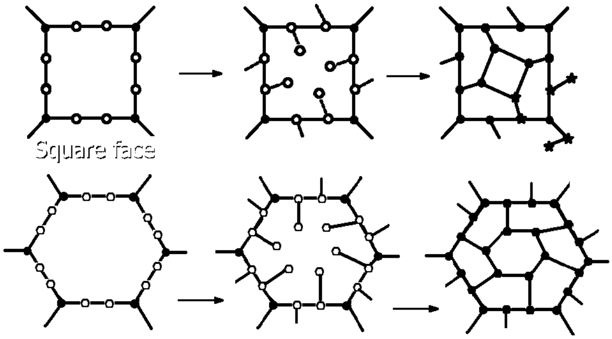

Figure 1. Capra map operation on the square and hexagonal face, respectively

Definition 2. Let *G* be a cyclic planar graph. Capra map operation is achieved as follows:

(i) insert two vertices on every edge of G;
(ii) add pendant vertices to the above inserted ones and
(iii) **c**onnect the pendant vertices in order (-1,+3) around the boundary of a face of G. By running these steps for every face/cycle of *G,* one obtains the Capra-transform of *G Ca(G)*, see Figure 1.

By iterating the Capra-operation on the hexagon (i.e. benzene graph C_6) and its Ca-transforms, a benzenoid series, as shown in Figures 2 and 3, can be designed. We will use the Capra-designed benzene series to calculate some connectivity indices (see below).

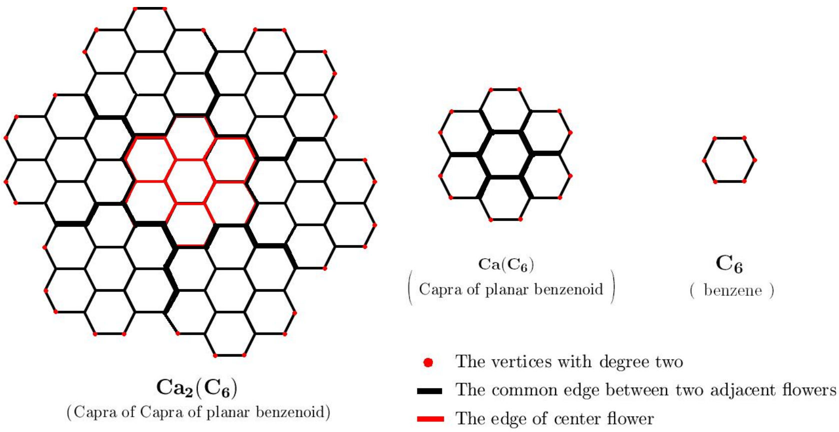

Figure 2. The first two graphs: *$Ca(C_6)$* and *$Ca_2(C_6)$* of the benzenoid family *$Ca_k(C_6)$*. Coloring is according to Definition 1.

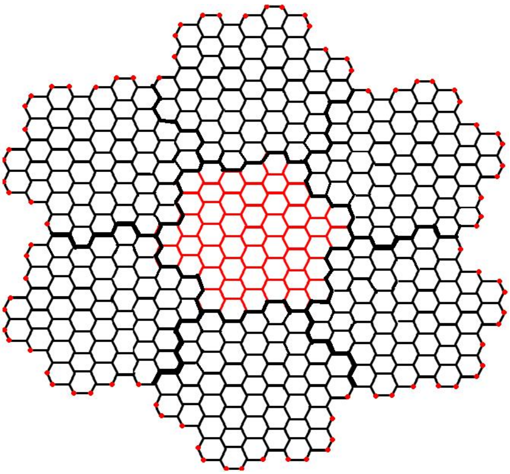

Figure 3. Graph $Ca_3(C_6)$ is the third member of Capra-designed planar benzenoid series.

Theorem 1. Let G=$Ca_k(C_6)$ $k\in N$ be the Capra-designed planar benzenoid series. Randić connectivity index is as follows:

$$\chi(Ca_k(C_6)) = \frac{2(7^k) + (4\sqrt{6}-1)3^{k-1} + 1}{2}$$

Proof. Let $G=Ca_k(C_6)$ $(k\geq 0)$ be the Capra-designed planar benzenoid series. The structure $Ca_k(C_6)$ collects seven times of structure $Ca_{k-1}(C_6)$ (we call "flower" the substructure $Ca_{k-1}(C_6)$ in the graph $Ca_k(C_6)$). Therefore, by a simple induction on k, the vertex set of $Ca_k(C_6)$ will have $7\times|V(Ca_k(C_6))|-6(2\times 3^{k-1}+1)$ members. Because, there are $3^{k-1}+1$ and 3^{k-1} common vertices between seven flowers $Ca_{k-1}(C_6)$ in $Ca_k(C_6)$, marked by full black color in the above figures. Also, by a similar inference, the edge set $E(Ca_k(C_6))$ has $7\times|E(Ca_k(C_6))|-6(2\times 3^{k-1}+1)$ members. Thus, there are 3^{k-1} and 3^{k-1} common edges, see Figures 2 and 3. Now by solving the recursive sequences, $n_k=|V(Ca_k(C_6))|$ and $e_k=|E(Ca_k(C_6))|$. Thus the size of vertex set and edge set of Capra-designed planar benzenoid series $Ca_k(C_6)$ $(k\geq 0)$ are equal to:

$$|V(Ca_k(C_6))|=2\times 7^k+3^{k+1}+1,\ |E(Ca_k(C_6))|=3(7^k+3^k).$$

Now, we can divide $V(Ca_k(C_6))$ and $E(Ca_k(C_6))$ to two and three partitions, respectively (See Definition 1). According to Figures 2 and 3, we see that the number of vertices with degree two of graph $Ca_k(C_6)$ (denoted by $v_2^{(k)}$) is equal to $6(3\left(\frac{v_2^{(k-1)}}{6}\right))-6.$ Therefore, we have $v_2^{(k)} = 3v_2^{(k-1)} - 6$ $= 3(3v_2^{(k-2)} - 6) - 6 = \ldots = 3^k v_2^{(0)} - 6\sum_{i=0}^{k-1} 3^i = \mathbf{3^{k+1} + 3}$ and $e_4^{(k)} = |E_4| = |E_4^*|$ $= v_2^{(k-1)} = \mathbf{3^k + 3}.$

Alternatively, the number of vertices of degree three is $|V_3| = |\{v \in V(Ca_k(C_6)) \,|\, d_v = 3\}| = 2(7^k - 1),$ (denoted by $v_3^{(k)}$).

On the other hand, according to the structure of Capra-designed planar benzenoid series, *G=Ca_k(C₆)*, $e_5^{(k)} = |E_5| = |E_6^*| = 2v_2^{(k)} - 2e_4^{(k)}.$ Thus, $e_5^{(k)} = 2v_2^{(k)} - 2v_2^{(k-1)} = \mathbf{4(3^k)}.$ The size of edge set E_5 and E_6^* is: $e_5^{(k)} = 2(3^{k+1} + 3 - 3^k - 3) = \mathbf{4(3^k)}.$ Thus, it is obvious that:

$$\begin{aligned} e_6^{(k)} = |E_6| = |E_9^*| &= 3\left(7^k + 3^k\right) - e_5^{(k)} - e_4^{(k)} \\ &= 3\times 7^k + 3^{k+1} - 4\times 3^k - 3^k - 3 \\ &= 3\times 7^k - 2\times 3^k - 3 \\ &= \mathbf{3(7^k - 2(3^{k-1}) - 1)}. \end{aligned}$$

Then, by using of size $V_2, V_3, E_4, E_4^*, E_5, E_6^*, E_6$ and E_9^*, we can compute Randić connectivity index of Capra-designed planar benzenoid series $G=Ca_k(C_6)$ as follows:

$$\begin{aligned} \chi(Ca_k(C_6)) &= \sum_{uv \in E(Ca_k(C_6))} \frac{1}{\sqrt{d(u)d(v)}} \\ &= \sum_{uv \in E_9^*} \frac{1}{\sqrt{d(u)d(v)}} + \sum_{uv \in E_6^*} \frac{1}{\sqrt{d(u)d(v)}} + \sum_{uv \in E_4^*} \frac{1}{\sqrt{d(u)d(v)}} \\ &= \frac{|E_9^*|}{\sqrt{9}} + \frac{|E_6^*|}{\sqrt{6}} + \frac{|E_4^*|}{\sqrt{4}} \\ &= \frac{3(7^k - 2(3^{k-1}) - 1)}{\sqrt{9}} + \frac{4(3^k)}{\sqrt{6}} + \frac{3^k + 3}{\sqrt{4}}. \end{aligned}$$

Finally, the Randić index of $Ca_k(C_6)$ is

$$\chi(Ca_k(C_6)) = \frac{\mathbf{2(7^k) + (4\sqrt{6} - 1)3^{k-1} + 1}}{\mathbf{2}}.$$

thus completing the proof of Theorem 1.

Theorem 2. Sum-connectivity index of Capra-designed planar benzenoid series $Ca_k(C_6)$ for integer k is equal to:

$$X(\mathbf{Ca_k}(\mathbf{C_6})) = \frac{3(\mathbf{3^{k-1}}+\mathbf{1})+\sqrt{6}(7^{\mathbf{k}}-\mathbf{1})}{\mathbf{2}} + \mathbf{3^{k-1}}\left(\frac{12\sqrt{5}-5\sqrt{6}}{5}\right).$$

Proof: By using the results from the above proof, it is immediate that

$$\begin{aligned}
X(Ca_k(C_6)) &= \sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u+d_v}} \\
&= \sum_{e=uv\in E_4} \frac{1}{\sqrt{d_u+d_v}} + \sum_{e=uv\in E_5} \frac{1}{\sqrt{d_u+d_v}} + \sum_{e=uv\in E_6} \frac{1}{\sqrt{d_u+d_v}} \\
&= \frac{|E_4|}{\sqrt{4}} + \frac{|E_5|}{\sqrt{5}} + \frac{|E_6|}{\sqrt{6}} \\
&= \frac{3^k+3}{\sqrt{4}} + \frac{4(3^k)}{\sqrt{5}} + \frac{3(7^k-2(3^{k-1})-1)}{\sqrt{6}}.
\end{aligned}$$

Thus $X(\mathbf{Ca_k}(\mathbf{C_6})) = \frac{3(\mathbf{3^{k-1}}+\mathbf{1})+\sqrt{6}(7^{\mathbf{k}}-\mathbf{1})}{\mathbf{2}} + \mathbf{3^{k-1}}\left(\frac{12\sqrt{5}-5\sqrt{6}}{5}\right).$

Theorem 3. Geometric-Arithmetic index and Atom-Bond connectivity index of Capra-designed planar benzenoid series are equal to (for all $k \in N$)

$$GA(Ca_k(C_6)) = 3(7^k) + \left(\frac{8\sqrt{6}}{5} - 1\right)3^k$$

$$ABC(Ca_k(C_6)) = 2(7^k) + (\frac{15\sqrt{2}-8}{2})3^{k-1} + (\frac{3\sqrt{2}-4}{2})$$

Proof. Let $G=Ca_k(C_6)$ $(k\geq 1)$ be Capra-designed planar benzenoid series. According to the proof of Theorem 1, we have $|E_6|=|E_9^*|=3(7^k-2(3^{k-1})-1)$, $|E_5|=|E_6^*|=4(3^k)$ and $|E_4|=|E_4^*|=3^k+3$. Thus, we can compute two connectivity topological indices geometric-arithmetic index and atom-bond connectivity index of $G=Ca_k(C_6)$ for any $k\geq 1$ as follows:

$$GA(Ca_k(C_6)) = \sum_{uv \in E(Ca_k(C_6))} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$$
$$= \sum_{e=uv \in E_4} \frac{2\sqrt{4}}{4} + \sum_{e=uv \in E_5} \frac{2\sqrt{6}}{5} + \sum_{e=uv \in E_6} \frac{2\sqrt{9}}{6}$$
$$= e_6^{(k)} \frac{6}{6} + e_5^{(k)} \frac{2\sqrt{6}}{5} + e_4^{(k)} \frac{4}{4}$$
$$= 3(7^k) + \left(\frac{8\sqrt{6}}{5} - 1\right)3^k$$

The geometric-arithmetic index of $Ca_k(C_6)$ is

$$GA(Ca_k(C_6)) = 3(7^k) + \left(\frac{8\sqrt{6}}{5} - 1\right)3^k.$$

Finally,

$$ABC(Ca_k(C_6)) = \sum_{uv \in E(Ca_k(C_6))} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$$
$$= \sum_{uv \in E_9^*} \frac{1}{\sqrt{d(u)d(v)}} + \sum_{uv \in E_6^*} \frac{1}{\sqrt{d(u)d(v)}} + \sum_{uv \in E_4^*} \frac{1}{\sqrt{d(u)d(v)}}$$
$$= e_6^{(k)} \sqrt{\frac{6-2}{9}} + e_5^{(k)} \sqrt{\frac{5-2}{6}} + e_4^{(k)} \sqrt{\frac{4-2}{4}}$$
$$= 3(7^k - 2(3^{k-1}) - 1)\frac{2}{3} + 4(3^k)\frac{\sqrt{2}}{2} + (3^k + 3)\frac{\sqrt{2}}{2}.$$

Therefore, atom-bond connectivity index of $Ca_k(C_6)$ will be

$$ABC(Ca_k(C_6)) = \mathbf{2(7^k) + (\frac{15\sqrt{2}-8}{2})3^{k-1} + (\frac{3\sqrt{2}-4}{2})}.$$

Here, the proof of Theorem 3 is completed.

ACKNOWLEDGMENTS

The authors are thankful to Professor Mircea V. Diudea, Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University for his precious support and suggestions.

REFERENCES

1. M. Randić, On characterization of molecular branching, *J. Amer. Chem. Soc.*, **1975**, *97,* 6609.
2. M. Ghorbani and M. Ghazi, *Digest. J. Nanomater. Bios.*, **2010**, *5(4),* 1107.
3. M. Ghorbani and M. Ghazi, *Digest. J. Nanomater. Bios.*, **2010**, *5(4),* 837.
4. J. Rada, O. Araujo, and I. Gutman, *Croat. Chem. Acta*, **2001**, *74,* 225.
5. B. Zhou and N. Trinajstić, On a novel connectivity index, *J. Math. Chem.,* **2009**, *46*, 1252.
6. B. Zhou and N. Trinajstić, On general sum-connectivity index, *J. Math. Chem.,* **2010**, *47*, 210.
7. D. Vukicevic and B. Furtula, *J. Math. Chem*., **2009**, *46,* 1369.
8. L. Xiao, S. Chen, Z. Guo and Q. Chen, *Int. J. Contemp. Math. Sci.,* **2010**, *5(45),* 2225.
9. Y. Yuan, B. Zhou and N. *Trinajstić, J. Math. Chem.,* **2010**, *47,* 833.
10. M.V. Diudea, Capra-a leapfrog related operation on maps, *Studia UBB Chemia*, **2003**, *48* (2), 3.
11. M.V. Diudea, Nanoporous carbon allotropes by septupling map operations. *J. Chem. Inf. Model*, **2005**, *45,* 1002.