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SECOND-CONNECTIVITY INDEX OF CAPRA-DESIGNED PLANAR BENZENOID SERIES $Ca_n(C_6)$

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ABSTRACT. The benzene is a key molecule in organic chemistry. In this paper, we focus on the structure of the *Capra*-designed planar benzenoid series $Ca_n(C_6)$ and compute the 2-connectivity index in the general case of this family of benzenoids.

Keywords: *Randić connectivity index, Sum-connectivity index, Benzenoid, Capra, Second connectivity index.*

INTRODUCTION

Let *G=(V,E)* be a simple connected graph with the vertex set *V(G)* and the edge set *E(G).* Molecular connectivity indices are related to the accessibility to the reaction centres. In identifying the accessibility perimeters, we have to recognize the atom degrees. The generalized connectivity index is the *m-connectivity* index, defined as:

$$^{m}\chi(G)=\sum_{v_{i_1}v_{i_2}..v_{i_{m+1}}}\frac{1}{\sqrt{d_{i_1}d_{i_2}..d_{i_{m+1}}}}$$

where $v_{i_1}v_{i_2}\dots v_{i_{m+1}}$ runs over all paths of length *m* in *G* and d_i is the degree of vertex $v_i \in V(G)$. In particular, 1-connectivity index (the original *Randić* index) can be written as

$$\chi(G)=\sum_{e=(i,j)\in E(G)}\frac{1}{\sqrt{d_i d_j}}$$

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The Randić Connectivity Index was introduced by *Milan Randić* [1, 2] in 1975. For more study, see references [3-9]. The *2-connectivity index* is defined as follows:

$$^{2}\chi(G) = \sum_{v_{i_1}v_{i_2}v_{i_3}} \frac{1}{\sqrt{d_{i_1}d_{i_2}d_{i_3}}}$$

The Randić and second-order connectivity indices (or 2-connectivity index) represents the molecular accessibility areas and volumes, respectively.

The *benzene* is a usual chemical molecule in chemistry with a distinctive structure. The benzene is a key molecule in chemistry and related sciences, with various applications in different fields.

We use the *Capra-designed operation* to generate new structures called benzoids. This operation was introduced by *M.V. Diudea* and used in many papers [10-19], see Figure 1.

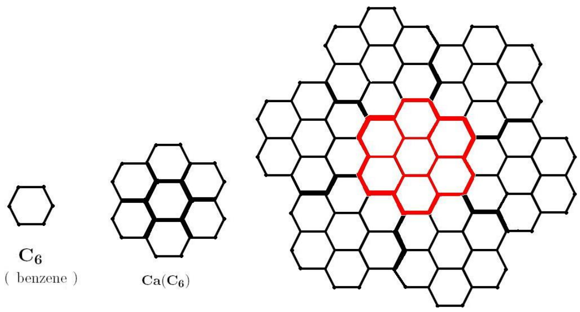

Figure 1. The first two graphs $Ca_1(C_6)$ and $Ca_2(C_6)$ from the Capra of planar benzenoid series and molecular graph benzene C_6=$Ca_0(C_6)$.

RESULTS AND DISCUSSION

Let d_{ij} denote the number of edges in G connecting vertices of degrees i and j; clearly, $d_{ij}=d_{ji}$. Define d_{ijk} as a number of 2-edges paths with 3 vertices of degree i, j and k, respectively. It is obvious that $d_{ijk} = d_{kji}$ and the number of 2-edge paths for all possible i, j and k is denoted by $d_2(G)$.

Theorem 1. [16] Consider the graph $G=Ca_k(C_6)$, $k \in N$ is the Capra-designed planar benzenoid series. Then Randić connectivity index $\chi(Ca_k(C_6))$ is equal to $\frac{2(7^k)+(4\sqrt{6}-1)3^{k-1}+1}{2}$.

Theorem 2. Second-connectivity index of $Ca_k(C_6)$ is computed as: $^{2}\chi(Ca_k(C_6)) = \frac{2\sqrt{3}}{3}7^k + \left(\frac{7\sqrt{2}}{6} - \frac{5\sqrt{3}}{18}\right)3^k + \left(\sqrt{3} - \frac{3\sqrt{2}}{2}\right).$

Proof of Theorem 2. Let $G=Ca_k(C_6)$ be the Capra-designed planar benzenoid series. Since, this graph has $2\times7^k+3^{k+1}+1$ vertices and $3\times7^k+3^{k+1}$ edges (denoted by n_k and e_k, respectively). At the first, we determine the number of 2-edge paths $d_2^{(k)}(G)$ in $G=Ca_k(C_6)$. So, we attend to d_{ijk} for every arbitrary vertices *i, j* and *k*; and obviously the number of d_{ijk} is dependent of the degree of vertex *j* (denoted by d_j). On the other hand, the number of 2-edge paths passing the vertex *j* of *G* is equal to $(d_j-1)+(d_j-2)+\ldots+(2)+(1)=\frac{d_j(d_j-1)}{2}$ and obviously $d_2^{(k)}(G)=\sum_{v\in V(G)}\frac{d_v(d_v-1)}{2}$. There are two partitions $V_2=\{v\in V(Ca_k(C_6))\,|\,d_v=2\}$ and $V_3=\{v\in V(Ca_k(C_6))\,|\,d_v=3\}$, with size $v_2^{(k)}=|V_2|=3^{k+1}+3$ and $v_3^{(k)}=|V_3|=2(7^k-1)$ respectively. Then,

$$\begin{aligned}
d_2^{(k)}(Ca_k(C_6)) &= \sum_{v\in V(Ca_k(C_6))}\frac{d_v(d_v-1)}{2}\\
&=\sum_{v\in V_3}\frac{3(3-1)}{2}+\sum_{v\in V_2}\frac{2(2-1)}{2}\\
&=3\times2(7^k-1)+1\times3(3^k+1)\\
&=6\times7^k+3^{k+1}+3
\end{aligned}$$

Now, according to the Capra-designed structure (Figure 2), we see that there exist two kinds of 2-edge paths $d_2^{(k)}(Ca_k(C_6))$: *internal 2-edge paths* and *external 2-edge paths*. Thus we have:

$$d_2^{(k)}(Ca_k(C_6)) = \underbrace{\underbrace{6(7^k)}_{6\zeta_k}}_{internal\ 2-edge\ paths} + \underbrace{\underbrace{3^{k+1}-3}_{v_2^{(k)}-6}}_{external\ 2-edge\ paths}$$

where ζ_k is the number of cycles with length six and is equal to 7^k. Alternatively, the number of internal 2-edge paths of $Ca_k(C_6)$ is equal to $d_{2\ (in)}^{(k)}=6\,\zeta_k=6(7^k)$. The number of external 2-edge paths of $Ca_k(C_6)$ is equal to $d_{2\ (ex)}^{(k)}=3^{k+1}-3$, being obtained from the sequence:

$$0,\ 6,\ 24,\ 6\times13,\ldots,\ d_{2\ (ex)}^{(k)}=6\left(\frac{d_{2\ (ex)}^{(k-1)}}{2}+1\right).$$

In proving theorem 2 we have to calculate the number of 2-edges paths $d_{223}^{(k)}$, $d_{333}^{(k)}$ from internal 2-edge paths and $d_{323}^{(k)}$, $d_{232}^{(k)}$ from external 2-edge paths:

$$d_2^{(k)}(Ca_k(C_6))=\underbrace{d_{223}^{(k)}+d_{333}^{(k)}}_{internal\ 2-edges\ paths}+d_{233}^{(k)}+\underbrace{d_{232}^{(k)}+d_{323}^{(k)}}_{external\ 2-edges\ paths}$$

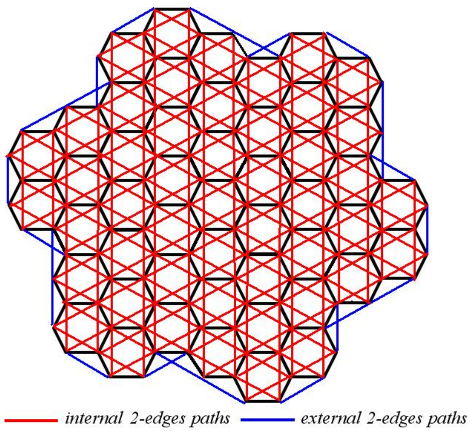

Figure 2. The internal 2-edges paths and external 2-edges paths of $Ca_2(C_6)$.

It is obvious that, in $C_6=Ca_0(C_6)$, $d_{223}^{(0)}=d_{323}^{(0)}=d_{232}^{(0)}=d_{233}^{(0)}=d_{333}^{(0)}=0$, $d_{222}^{(0)}=6$ and

$$^2\chi(Ca_0(C_6))=\frac{6}{\sqrt{2\times2\times2}}=2.1213$$

Next, for $Ca_1(C_6)$, $d_{223}^{(1)}=2\times6$, $d_{323}^{(1)}=0$, $d_{232}^{(1)}=6$, $d_{233}^{(1)}=2\times6$ and $d_{333}^{(1)}=18$. Thus

$$^2\chi(Ca_1(C_6))=\frac{12}{\sqrt{2\times2\times3}}+\frac{6}{\sqrt{2\times3\times2}}+\frac{12}{\sqrt{2\times3\times3}}+\frac{0}{\sqrt{3\times2\times3}}+\frac{18}{\sqrt{3\times3\times3}}=11.4886.$$

Now, by simple calculation and induction on $n=1,2,3,\ldots,k$, (see Figure 1., 2. and 3.) we show that for $G=Ca_k(C_6)$

$$d_{223}^{(0)}=0,\ d_{223}^{(1)}=12,\ d_{223}^{(2)}=24,\ d_{223}^{(3)}=2(3^3+3)=60,\ \ldots,\ \underbrace{d_{223}^{(k)}}_{internal}=2(3^k+3)=2e_4^{(k)}.$$

$$d_{323}^{(0)}=0,\ d_{323}^{(1)}=0,\ d_{323}^{(2)}=12,\ d_{323}^{(3)}=24,\ \ldots,\ \underbrace{d_{323}^{(k)}=v_2^{(k)}-2e_4^{(k)}}_{external}=3^{k+1}+3-2(3^k+3)=3^k-3.$$

$$d_{232}^{(0)}=0,\ d_{232}^{(1)}=6,\ d_{232}^{(2)}=12,\ d_{232}^{(3)}=6(\frac{12}{2}-1)=30,\ \ldots,\ d_{232}^{(k)}=6(\frac{d_{232}^{(k-1)}}{2}-1)=3d_{232}^{(k-1)}-6=3^k+3.$$

$$d_{233}^{(0)}=0,\ d_{233}^{(1)}=\underbrace{0}_{ex}+\underbrace{2\times6}_{in}=12,\ d_{233}^{(2)}=\underbrace{2\times6}_{ex}+\underbrace{6\times6}_{in}=48,\ d_{232}^{(3)}=\underbrace{8\times6}_{ex}+\underbrace{18\times6}_{in}=156,$$

$$\ldots,\ d_{233}^{(k)}=d_{233(ex)}^{(k)}+d_{233(in)}^{(k)}=6(3^k-1)$$

where

$$\begin{cases} d_{233\,(ex)}^{(k)}=d_{323\,(ex)}^{(k)}-d_{232\,(ex)}^{(k)}=3^{k+1}-3-(3^k+3)=6(3^{k-1}-1) \\ d_{233\,(in)}^{(k)}=6(\frac{d_{233\ \ (in)}^{(k-1)}}{2})=3d_{233\ \ (in)}^{(k-1)}=4(3^k) \end{cases}$$

$d_{333}^{(0)}=0,\quad d_{333}^{(1)}=18,\quad d_{333}^{(2)}=228,\quad d_{333}^{(3)}=1866,\quad \ldots,$

$$\underbrace{d_{333}^{(k)}}_{internal}=d_2^{(k)}-d_{233\,(ex)}^{(k)}-d_{233\,(in)}^{(k)}-d_{232\,(ex)}^{(k)}-d_{323\,(ex)}^{(k)}-d_{223\,(in)}^{(k)}$$

$$=6(7^k)+3^{k+1}-3-2(3^k)-6-3^k+3-6(3^k)+6-3^k-3=6\times 7^k-7(3^k)-3$$

In totally,

$$d_{ijk}^{(k)}=\begin{cases}6(7^k)-7(3^k)-3 & ijk=333\\ 2e_4^{(k)}=2(3^k+3) & ijk=223\end{cases}\ \text{internal } 2-\text{edge paths}$$
$$\quad 6(3^{k-1}-1)+4(3^k)=6(3^k-1) \qquad ijk=233$$
$$\begin{cases}v_2^{(k)}-2e_4^{(k)}=3^k-3 & ijk=323\\ 3^k+3 & ijk=232\end{cases}\ \text{external } 2-\text{edge paths}$$

where $e_4^{(k)}=3^k-3$ is the number of edge of $Ca_k(C_6)$ with end-point and first-point of degree 2. Therefore:

$${}^2\chi(Ca_k(C_6))=\sum_{v_{i_1}v_{i_2}v_{i_3}}\frac{1}{\sqrt{d_{i_1}d_{i_2}d_{i_3}}}$$
$$=\frac{2(3^k+3)+3^k+3}{\sqrt{12}}+\frac{3^k-3+6(3^k)-6}{\sqrt{18}}+\frac{6(7^k)-7(3^k)-3}{\sqrt{27}}$$
$$=\frac{3^{k+1}+9}{6}\sqrt{3}+\frac{7(3^k)-9}{6}\sqrt{2}+\frac{6(7^k)-7(3^k)-3}{9}\sqrt{3}$$
$$=\frac{(3^{k+2}+27+12(7^k)-14(3^k)-6)\sqrt{3}+(7(3^{k+1})-27)\sqrt{2}}{18}$$
$$=\frac{((12(7^k)-5(3^k)+21)\sqrt{3}+(7(3^{k+1})-27)\sqrt{2})}{18}.$$

The second-connectivity index of $Ca_k(C_6)$ is equal to

$${}^2\chi(Ca_k(C_6))=\frac{2\sqrt{3}}{3}7^k+\left(\frac{7\sqrt{2}}{6}-\frac{5\sqrt{3}}{18}\right)3^k+\left(\sqrt{3}-\frac{3\sqrt{2}}{2}\right).$$

Thus, we completed the proof of Theorem 2.

We can use formula for ${}^2\chi(Ca_k(C_6))$ to compute some numerical examples:

$${}^2\hat{\chi}(Ca_k(C_6))=1.1547(7^k)+1.1688(3^k)-0.3892.$$

Examples for ${}^2\chi(Ca_k(C_6))$ for $k=1, 2, 3, 4, 5, 10, 20, 30, 40, 50, 100$ are given in Table 1.

Table 1. Values of second-connectivity index $^{2}\chi(Ca_k(C_6))$

k	Number of Vertices	Number of edges	2-connectivity index
1	*24*	*30*	*11. 2001*
2	*123*	*174*	*66. 7103*
3	*768*	*1110*	*427. 2305*
4	*5046*	*7446*	*2866. 7183*
5	*34344*	*51150*	*19690. 6721*
10	*565127646*	*847602894*	*326243186. 1023*
20	*1. 5958454306×10^17*	*2. 3937680935×10^17*	*9. 2136133969×10^16*
30	*4. 5078680582×10^25*	*6. 6718020873×10^25*	*2. 602617623×10^25*
40	*1. 2733611522×10^34*	*1. 9100417283 ×10^34*	*7. 3517506121 ×10^33*
50	*3. 596330085×10^42*	*5. 3953951279 ×10^42*	*2. 0766875847 ×10^42*
100	*6. 4689530192×10^84*	*9. 7034295289 ×10^84*	*6. 4689530192 ×10^84*

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