COMPUTING SANSKRUTI INDEX OF CAPRA-DESIGNED
PLANAR BENZENOID SERIES $Ca_k(C_6)$

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Abstract: Let $G = (V, E)$ be a molecular graph, such that vertices represent atoms and edges are chemical bonds. The Sanskruti index of a graph G is a topological index was defined as $S(G) = \sum_{uv \in E(G)} (\frac{S_u S_v}{S_u + S_v - 2})^3$ where S_u is the summation of degrees of all neighbors of vertex u in G . This connectivity indices is very important and they has a prominent role in chemistry. In this paper, we focus on the structure of Capra-designed planar benzenoid series $Ca_k(C_6)$ ($k \geq 0$) and compute on this above topological descriptor.

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1. Introduction and Preliminaries

Let $G = (V; E)$ be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge sets of it are represented by $V = V(G)$ and $E = E(G)$, respectively. In chemical graphs, the vertices correspond to the atoms of the molecule, and the edges represent to the chemical bonds. Also, 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".

The chemical graph theory is an important branch of mathematical chemistry. In this branch, there are many molecular descriptors (or Topological Indices), that have very useful properties to study of chemical molecules. A topological index is a real number associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry. A connected graph is a graph such that there is a path between all pairs of vertices.

The Sanskruti index $S(G)$ of a graph G is defined as follows (see [1]-[6]):

$$S(G) = \sum_{uv \in E(G)} \left(\frac{S_u S_v}{S_u + S_v - 2} \right)^3.$$

where S_u is the summation of degrees of all neighbors of vertex u in G .

In chemistry, physics and nanoscience, there are especially symmetric structures. Such molecular graphs are Capra-designed planar benzenoids. Capra Ca map operation (also called Septupling S_1) is a method of drawing and modifying the covering of a polyhedral structure, introduced by M.V. Diudea (see [7],[8]) and used in many papers (see the references [9]-[20] and a detailed example is given in Figure 1.)

In this paper, we applied Capra operation on the benzene molecular graph C_6 to design planar benzenoid structures; the k -iterated benzenoids are denoted $Ca_k(C_6)$. The first members of this series are shown in following figures.

Within this paper, we focused on connectivity topological indices and compute the Sanskruti index of molecular graphs related to Coronene $Ca(C_6)$ planar benzenoid structure. Our notation is standard and mainly taken from ref-s. [21]-[23].

Figure 1: An example of Capra map operation on the hexagon face. Since Capra of planar benzenoid series has a very remarkable structure, we lionize it.

Figure 2: The first two graphs $Ca(C_6)$ and $Ca_2(C_6)$ from the Capra of planar benzenoid series, together with the molecular graph of benzene C_6 . Benzene is equivalent with $Ca_0(C_6)$.

2. Main Results and Discussion

The aim of this section is to obtain a closed formula of Sanskruti index $S(G)$ of general representation of Capra-designed planar benzenoid series $Ca_k(C_6)$ and we have following theorem, immediately.

Theorem 2.1. Consider the graph $G = Ca_k(C_6)$ ($k \geq 1$) as the iterative Capra-designed planar benzenoid series. Then:

$$S(VPHX[m, n]) = -\frac{87714218531}{175616000}m + \frac{4782969}{4096}mn.$$

Figure 3: Graph $\text{Ca}_3(\text{C}_6)$ is the third member of Capra-designed planar benzenoid series $\text{Ca}_k(\text{C}_6)$.

Proof. Consider the Capra of planar benzenoid series $G = \text{Ca}_k(\text{C}_6)$ ($k \geq 1$). By construction, the structure $\text{Ca}_k(\text{C}_6)$ collects seven times of structure $\text{Ca}_{k-1}(\text{C}_6)$ (we call "flower" the substructure $\text{Ca}_{k-1}(\text{C}_6)$ in the graph $\text{Ca}_k(\text{C}_6)$). Therefore, by simple induction on k , the vertex set of $\text{Ca}_k(\text{C}_6)$ will have $7 \times |V(\text{Ca}_k(\text{C}_6))| - 6(2 \times 3^{k-1} + 1)$ members. Thus the number of vertices/atoms in this benzenoid system is equal to

$$n_k = |V(\text{Ca}_k(\text{C}_6))| = 2 \times 7^k + 3^{k+1} + 1 \quad (\forall k \geq 0)$$

and alternatively the number of edges/bonds is $e_k = |E(\text{Ca}_k(\text{C}_6))| = 3(7^k + 3^k)$.

There are two partitions $V_2 = \{v \in V(G) | d_v = 2\}$ and $V_3 = \{v \in V(G) | d_v = 3\}$ of $V(\text{Ca}_k(\text{C}_6))$, since the degree of an arbitrary vertex/atom of a molecular

graph is equal to 2 or 3. Next, these partitions imply that $E(TUAC_6[m, n])$ can be divided in three partitions $E_6 = \{u, v \in V(Ca_k(C_6)) | d_u = d_v = 3\}$, $E_5 = \{u, v \in V(G) | d_u = 3 \& d_v = 2\}$, and $E_4 = \{u, v \in V(Ca_k(C_6)) | d_u = d_v = 2\}$.

According to Figures 2 and 3, we see that the number of vertices of degree two in the graph $Ca_k(C_6)$ (we denote by $v_2^{(k)}$) is equal to $v_2^{(k)} = 6 \times 3(\frac{v_2^{(k-1)}}{6}) - 6 = 3^{k+1} + 3$. Also, obviously, $v_3^{(k)} = 2(7^k - 1)$ and $e_4^{(k)} = |E_4| = v_2^{(k-1)} = 3^k + 3$.

On the other hand, according to the structure of Capra planar benzenoid series $Ca_k(C_6)$, there are $2v_2^{(k)}$ edges, such that the first-point of them is a vertex with degree two. Among these edges, there exist $V_2^{(k-1)}$ edges, of which first and end point of them have degree 2 (the members of E_4).

Thus, the size of edge set E_5 is equal to

$$e_5^{(k)} = |E_5| = 2v_2^{(k)} - 2e_4^{(k)} = 2v_2^{(k)} - 2v_2^{(k-1)} = 2(3^{k+1} + 3 - 3^k - 3) = 4(3^k).$$

So, $2e_4^{(k)}$ vertices/atoms with degree two have $S_v = 2 + 3 = 5$ and other $(v_2^{(k)} - 2e_4^{(k)}) = 3^k - 3$ have $S_v = 3 + 3 = 6$.

From figures, it is easy to see that there are $e_4^{(k)}$ vertices as degree 3, such that the summation of their adjacent vertices is equal to $7 (= 2 + 2 + 3)$.

On the other hand, there are $e_5^{(k)} - 2e_4^{(k)} (= 2(3^k) - 6)$ vertices as degree 3 have $S_v = 2 + 3 + 3 = 8$.

From above results, it is obvious that for all other vertices/atoms $v_3^{(k)} - (3^k + 3 + 2(3^k) - 6) = 2(7^k) - 3^{k+1} + 1$ (which belong to V_3), we have $S_v = 9$.

Therefore $\forall k \geq 1$, we have following computations for the Sanskruti index of Capra-designed planar benzenoid series $G = Ca_k(C_6)$:

$$\begin{aligned} S(Ca_k(C_6)) &= \sum_{uv \in E(G)} \left(\frac{S_u S_v}{S_u + S_v - 2} \right)^3 \\ &= \sum_{u_2 v_2 \in E_4} \left(\frac{S_u S_v}{S_u + S_v - 2} \right)^3 + \sum_{u_2 v_3 \in E_5} \left(\frac{S_u S_v}{S_u + S_v - 2} \right)^3 \\ &\quad + \sum_{u_3 v_3 \in E_6} \left(\frac{S_u S_v}{S_u + S_v - 2} \right)^3 \\ &= (3^k + 3) \left(\frac{5.5}{5 + 5 - 2} \right)^3 + (3^k - 3) \left(\frac{5.7}{5 + 7 - 2} \right)^3 \\ &\quad + (3^k - 3) \left(\frac{5.8}{5 + 8 - 2} \right)^3 + (3^k + 9) \left(\frac{6.7}{6 + 7 - 2} \right)^3 \\ &\quad + \left(\frac{2(3^k) - 6}{2} \right) \left(\frac{6.8}{6 + 8 - 2} \right)^3 + (3^k + 3) \left(\frac{7.9}{7 + 9 - 2} \right)^3 \end{aligned}$$

$$\begin{aligned}
& + \left(\frac{2(3^k - 3)}{2}\right)\left(\frac{8.8}{8 + 8 - 2}\right)^3 + 2(3^k - 3)\left(\frac{8.9}{8 + 9 - 2}\right)^3 \\
& + (3(7^k) - 2(3^{k-1} + 3))\left(\frac{9.9}{9 + 9 - 2}\right)^3.
\end{aligned}$$

Thus,

$$\begin{aligned}
S(Ca_k(C_6)) = & \frac{18962048164233}{29218112000}3^k - \frac{37374074037717}{233744896000} \\
& + \frac{1594323}{4096}7^k - \frac{531441}{2048}3^{k-1}.
\end{aligned}$$

The proof of theorem is completed. $\square$

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