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On the Sanskruti Index of Circumcoronene Series of Benzenoid

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Abstract

Let $G=(V;E)$ be a simple connected graph. The sets of vertices and edges of G are denoted by $V=V(G)$ and $E=E(G)$, respectively. In such a simple molecular graph, vertices represent atoms and edges represent bonds. The Sanskruti index $S(G)$ is a topological index was defined as $S(G)=\sum_{uv\in E(G)}\left(\frac{S_uS_v}{S_u+S_v-2}\right)^3$ where S_u is the summation of degrees of all neighbors of vertex u in G. The goal of this paper is to compute the Sanskruti index for circumcoronene series of benzenoid.

Keywords

Sanskruti Index, Molecular Graph, Circumcoronene Series of Benzenoid

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. Note that hydrogen atoms are often omitted. 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.

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [1] [2] [3]. This theory had an important effect on the development of the chemical sciences.

In mathematical chemistry, numbers encoding certain structural features of organic molecules and derived from the corresponding molecular graph, are called graph invariants or more commonly topological indices.

Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry. One of the best known and widely used is the connectivity index, introduced in 1975 by Milan Randić [4], who has shown this index to reflect molecular branching.

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

where d_u denotes G degree of vertex u. One of the important classes of connectivity indices is Sanskruti index $S(G)$ defined as [5]

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

Here our notation is standard and mainly taken from standard books of chemical graph theory [1] [2] [3].

2. Main Results and Discussions

In this section, we compute the Sanskruti index $S(G)$ for circumcoronene series of benzenoid. The circumcoronene series of benzenoid is family of molecular graph, which consist several copy of benzene C_6 on circumference. The first terms of this series are $H_1=\text{benzene}$, $H_2=\text{coronene}$, $H_3=\text{circumcoronene}$, $H_4=\text{circumcircumcoronene}$, see **Figure 1** and **Figure 2** where they are shown, also for more study and historical details of this benzenoid molecular graphs see the paper series [6]-[15].

At first, consider the circumcoronene series of benzenoid H_k for all integer number $k\geq 1$. From the structure of H_k (**Figure 2**) and references [17]-[23], one can see that the number of vertices/atoms in this benzenoid molecular

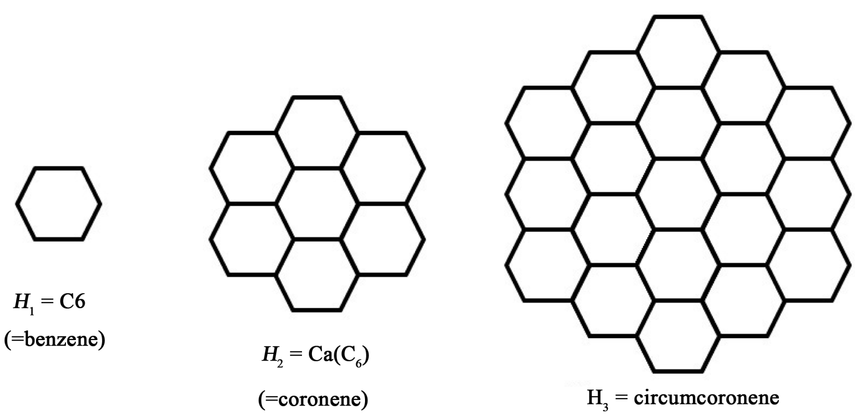

Figure 1. The three graphs H_1, H_2, H_3 of the circumcoronene series of benzenoid [16].

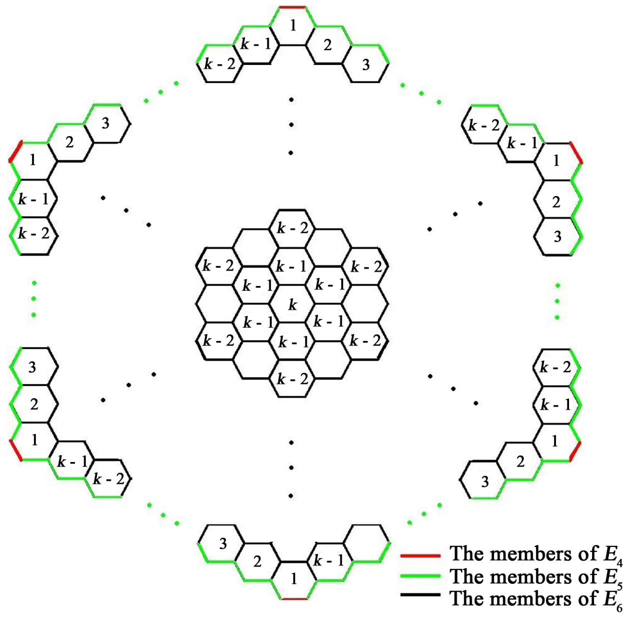

Figure 2. The general representation H_k of the circumcoronene series of benzenoid [16].

graph is equal to $|V(H_k)| = 6k^2$ and the number of edges/bonds is equal to $|E(H_k)| = \frac{3\times 6k(k-1)+2\times 6k}{2} = 9k^2-3k$. Because, the number of vertices/atoms as degrees 2 and 3 are equal to $6k$ and $6k(k-1)$ and in circumco- ronene series of benzenoid molecule, there are two partitions $V_2 = v \in V(G) | d_v = 2$ and $V_3 = v \in V(G) | d_v = 3$ of vertices. These partitions imply that there are three partitions E_4, E_5 and E_6 of edges set of molecule H_k with size 6, $12(k-1)$ and $9k^2-15k+6$, respectively. Clearly, we mark the members of E_4, E_5 and E_6 by red, green and black color in Figure 2.

From Figure 2, one can see that the summation of degrees of vertices of molecule benzenoid H_k are in four types, as follow:

- $S_v = S_u = 2+3 = 5$ for $u, v \in V_2$ and $uv \in E_4$
- $S_u = d_v + d_v = 6$ for $u \in V_2, v \in V_3$ and $uv \in E_5$
- $S_u = d_v + d_v + 3 = 7$ for $u \in V_3, v \in V_2$ and $uv \in E_5$
- $S_u = S_v = d_v + d_u + 3 = 9$ for $u, v \in V_3$ and $uv \in E_6$

So, the Sanskruti index for circumcoronene series of benzenoid $H_k(k \geq 1)$ will be

$$\begin{aligned} S(H_k) &= \sum_{uv\in E(G)} \left(\frac{S_u S_v}{S_u + S_v - 2}\right)^3 \\ &= (6)\left(\frac{5\times 5}{5+5-2}\right)^3 + (6)\left(\frac{5\times 7}{5+7-2}\right)^3 + \left(2\times 6(k-2)\right)\left(\frac{6\times 7}{6+7-2}\right)^3 \\ &\quad + \left(6(k-1)\right)\left(\frac{7\times 9}{7+9-2}\right)^3 + \left(9k^2-21k+12\right)\left(\frac{9\times 9}{9+9-2}\right)^3 \\ &= \frac{6561}{8}k^2 - \frac{5141425023}{4499456}k + \frac{6499681847}{40495104}. \end{aligned}$$

3. Conclusion

In this paper, we discuss the Sanskruti index. We consider the molecular graph "circumcoronene series of benzenoid" and we compute its Sanskruti index.

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