Computing Sanskruti index of the Polycyclic Aromatic Hydrocarbons

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ABSTRACT

Among topological descriptors topological indices are very important and they have a prominent role in chemistry. One of them is Sanskruti index was introduced by Hosamani and defined as

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

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

In this paper we compute this new topological index for Polycyclic Aromatic Hydrocarbons \( \text{PAH}_k \).

Introduction

Let \( G = (V; E) \) be a simple molecular graph without direction, multiple edges and loops, and 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 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”.

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 (Estrada, Torres, Rodriguez, & Gutman, 1998; Gutman & Trinajstic, 1972; Tabar, 2009; Todeschini & Consonni, 2000; West, 1996). 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. In other words, if \( G \) be the connected graph, then we can introduce many connectivity topological indexes for it, by distinct and different definition. A connected graph is a graph such that there is a path between all pairs of vertices. One of the best known and widely used is the connectivity index, introduced in 1975 by Randic (1975), who has shown this index to reflect molecular branching and defined as follows:

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

where \( d_u \) denotes \( G \) degree of vertex \( u \).

The Sanskruti index \( S(G) \) of a graph \( G \) is defined in (Hosamani, 2016) as follows:

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

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

Main result

In this section, we computed the Sanskruti index \( S(G) \) of Polycyclic Aromatic Hydrocarbons \( \text{PAH}_k \). A two-dimensional lattice of Polycyclic Aromatic Hydrocarbon (\( \text{PAH}_k \)) is shown in Figure 2. It has \( 6k^2 + 6k \) vertices and \( 9k^2 + 3k \) edges.

Polycyclic Aromatic Hydrocarbons \( \text{PAH}_k \) are a group of more than 100 different chemicals that are formed during the incomplete burning of garbage, gas, oil, coal or other organic materials. Some \( \text{PAH}_k \) are manufactured. These \( \text{PAH}_k \) usually exist as, colorless, white, and pale yellow-green solids. The \( \text{PAH}_k \) discussed in this paper is a family of hydrocarbons containing several copies of benzene on circumference. A member of this family for \( k = 2 \) is shown in Figure 1 and a general representation is shown in Figure 2.
In (Farahani, 2013a, 2013b, 2013c, 2014, 2015a, 2015b; Farahani & Gao, 2015a, 2015b; Farahani & Rajesh Kanna, 2015a, 2015b; Farahani, Gao, & Rajesh Kanna, 2015a, 2015b; Farahani, Jamil, & Rajesh Kanna, 2016; Farahani, Rehman, Jamil, & Lee, 2016; Farahani, Jamil, Rajesh Kanna and Kumar, 2016a, 2016b; Gao & Farahani, 2015; Jamil, Farahani, Ali Malik, & Imran, 2016; Jamil, Farahani, & Kanna, 2016; Jamil, Rehman, Farahani, & Lee, 2016; Lee, Jamil, Farahani, & Rehman, 2016; Li et al., 2017; Woodard & Snedeker, 2001; Yan, Li, Farahani, Imran, & Rajesh Kanna, 2016) some topological indices of molecular graphs Polycyclic Aromatic Hydrocarbons PAH\(_k\) are computed. In this paper, we continue this work to compute the Sanskruti index of Polycyclic Aromatic Hydrocarbons PAH\(_k\).

**Theorem 1:** Consider the graph of Polycyclic Aromatic Hydrocarbon PAH\(_k\), then the Sanskruti index of PAH\(_k\) is equal to:

\[
S(PAH_k) = \frac{6561}{8} k^2 - \frac{7407927}{128000} k + \frac{73155}{1024}.
\]

**Proof:** From Figure 2, we noticed that in the structure of PAH\(_k\) vertices have degrees 1 or 3. We denote the sets of vertices with degrees 1 and 3 as \(V_1 = \{v \in V(G)|d_v = 1\}\) and \(V_3 = \{v \in V(G)|d_v = 3\}\). From \(V_1\) and \(V_3\), we have edge partitions \(E_4 = \{uv \in E(PAH_k)|d_u + d_v = 4\}\) and \(E_6 = \{uv \in E(PAH_k)|d_u + d_v = 6\}\) and \(|E_4| = 6k\), \(|E_6| = 9k^2 - 3k\).

Clearly, the sum of degrees of vertices for each edge of PAH\(_k\) is as follows:

- There are 6k edges \(e = uv\) for which, \(S_u = 3, S_v = 7\) when \(u \in V_1, v \in V_3\) and \(uv \in E_4\).
- There are 6 edges \(e = uv\) for which, \(S_u = S_v = 7\) when \(uv \in V_3\) and \(uv \in E_6\).
- There are \(12(k-1)\) edges \(e = uv\) for which, \(S_u = 7, S_v = 9\) when \(uv \in V_1\) and \(uv \in E_6\).
- There are \(9k^2 - 15k + 6\) edges \(e = uv\) for which, \(S_u = S_v = 9\) when \(uv \in V_3\) and \(uv \in E_6\).
From the above calculation, now we can obtain the required result.

\[
S(\text{PAH}_k) = \left( \frac{S_u S_v}{S_u + S_v - 2} \right)^3,
\]

\[
= \sum_{uv \in E_k} \left( \frac{S_u S_v}{S_u + S_v - 2} \right)^3 + \sum_{uv \in E_k} \left( \frac{S_u S_v}{S_u + S_v - 2} \right)^3
+ \sum_{uv \in E_k} \left( \frac{S_u S_v}{S_u + S_v - 2} \right)^3
= \sum_{uv \in E_k} \left( \frac{3 \times 7}{3 + 7 - 2} \right)^3 + \sum_{uv \in E_k} \left( \frac{7 \times 7}{7 + 7 - 2} \right)^3
+ \sum_{uv \in E_k} \left( \frac{7 \times 9}{9 + 9 - 2} \right)^3 + \sum_{uv \in E_k} \left( \frac{9 \times 9}{9 + 9 - 2} \right)^3
= \frac{6561}{8} \kappa^2 - \frac{74079927}{128000} \kappa + \frac{73155}{1024}.
\]

So, the proof is complete.

**Disclosure statement**

No potential conflict of interest was reported by the authors.

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